DOE-FIU Cooperative Agreement Annual Research Review – FIU Year 2

Tuesday, September 27, 2022		
9:30 - 9:35 am EDT	Kick-Off /Welcoming Remarks (DOE-EM)	Kurt Gerdes (Director, Technology Development) – DOE EM-3.2
9:35 - 9:40 am EDT	Welcoming Remarks (DOE-LM)	Leonel Lagos on behalf of DOE Office of Legacy Management
9:40 - 10:00 am EDT	Projects 4 & 5: STEM Workforce Development and Training	FIU, DOE HQ (EM & LM), SRNL, PNNL, WIPP, SRS, ORP, LBNL, WRPS, INL, Grand Junction
BREAK		
11:00 - 12:00 pm EDT	Projects 4 & 5 (cont'd): STEM Workforce Development and Training	FIU, DOE HQ (EM & LM), SRNL, PNNL, WIPP, SRS, ORP, LBNL, WRPS, INL, Grand Junction
BREAK		
1:00 - 2:30 pm EDT	Project 1: Chemical Process Alternatives for Radioactive Waste	FIU, DOE HQ, PNNL, WRPS, SRNL, SRS
2:30 - 4:00 pm EDT	Project 3: Waste and D&D Engineering & Technology Development	FIU, DOE HQ, SRNL, PNNL, LBNL, INL, ANL
Wednesday, September 28, 2022		
10:00 - 11:30 am EDT	Project 2: Environmental Remediation Science & Technology	FIU, DOE HQ, SRNL, PNNL, ORNL, LANL, CBFO
11:30 - 1:00 pm EDT	Wrap Up (FIU Projects 1, 2, 3, 4 & 5)	FIU, DOE HQ (EM & LM)

PROJECT 3

Waste and D&D Engineering & Technology Development

FIU Personnel and Collaborators

Project Manager: Leonel Lagos

Faculty/Researcher: Himanshu Upadhyay, Joseph Sinicrope, Walter Quintero, Clint Miller, Santosh Joshi, John Dickson, Mellissa Komninakis, Kexin Jiao, Masudur Siddiquee

DOE Fellows/Students: Roger Boza, David Mareno, Aurelien Meray, Adrian Muino Ayala, Christian Lopez, Christian Dau, Derek Gabaldon, Philip Moore

DOE-EM: Dinesh Gupta, Genia McKinley, Jean Pabon, Jonathan Kang, Douglas Tonkay, Jennifer McCloskey

SRNL: Jennifer Wohlwend, Connor Nicholson, Nick Groden, Aaron Washington, *Tristan Simoes-Ponce, Carol Eddy-Dilek

PNNL: Vicky Freedman, Rob Mackley

INL: Rick Demmer

LBNL: Haruko Wainwright

*Former staff/student contributors

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Project Tasks and Scope

TASK 1: WASTE INFORMATION MANAGEMENT SYSTEM (WIMS) (HQ)	
Subtask 1.1	WIMS System Administration - Database Management, Application Maintenance & Performance Tuning
Subtask 1.2	Waste Stream Annual Data Integration
Subtask 1.3	Cyber Security of WIMS Infrastructure
TASK 2: D&D SUPPORT TO DOE EM FOR TECHNOLOGY INNOVATION, DEVELOPMENT, EVALUATION AND DEPLOYMENT	
Subtask 2.1	Development of Uniform Testing Protocols and Standard Specifications for Dust Suppressant Technologies in Support of Open-Air Demolition during D&D
Subtask 2.2	Applications of Intumescent Foams and Other Fire-Retardant Materials to Mitigate Contaminant Release during Nuclear Pipe Dismantling and other D&D Activities
Subtask 2.3	Certifying Fixative Technology Performance when Exposed to Impact Stressors as Postulated in Contingency Scenarios Highlighted in Safety Basis Documents
Subtask 2.4	Multi-functional 3D Polymer Framework for Mercury Abatement

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Project Tasks and Scope

TASK 3: D&D KNOWLEDGE MANAGEMENT INFORMATION TOOL (KM-IT) (HQ, SRNL, INL, ANL)	
Subtask 3.4	Content Management
Subtask 3.5	Marketing and Outreach
Subtask 3.6	D&D KM-IT System Administration
Subtask 3.7	D&D KM-IT System Administration
Subtask 3.8	KM-IT Tech Talks
TASK 6: AI FOR EM PROBLEM SET (D&D): STRUCTURAL HEALTH MONITORING OF D&D FACILITY TO IDENTIFY CRACKS AND STRUCTURAL DEFECTS FOR SURVEILLANCE AND MAINTENANCE (SRNL)	
Subtask 6.5	Design & Development of Machine Learning and Deep Learning Models to Identify and Locate Cracks in D&D Mockup Facility
Subtask 6.6	Design & Development of a Mobile Application to Deploy Machine Learning and Deep Learning Models on the iOS Devices at SRS
Subtask 6.7	Research and Prototype Deployment of a Web Service API framework for AI Deep Learning Model (NEW)

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Project Tasks and Scope

TASK 7: AI FOR EM PROBLEM SET (SOIL AND GROUNDWATER) - EXPLORATORY DATA ANALYSIS AND MACHINE LEARNING MODEL FOR HEXAVALENT CHROMIUM (CR [VI]) CONCENTRATION IN 100-H AREA (PNNL)	
Subtask 7.2	Data Pre-processing and Exploratory Data Analysis to Evaluate the Chromium Concentration in the Samples
Subtask 7.3	Groundwater and Surface Water Spatiotemporal Relationship Identification
TASK 8: AI FOR EM PROBLEM SET (SOIL AND GROUNDWATER) - DATA ANALYSIS AND VISUALIZATION OF SENSOR DATA FROM WELLS AT THE SRS F-AREA USING MACHINE LEARNING (LBNL, SRNL)	
Subtask 8.4	Data Ingestion/Communication Module Development for the AI/ML System
Subtask 8.5	Development of the AI/ML-Based System to Perform Predictive Analytics using Datasets containing Time-Series and Imagery Data from Sensors

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Task 1

Waste Information Management System (WIMS)

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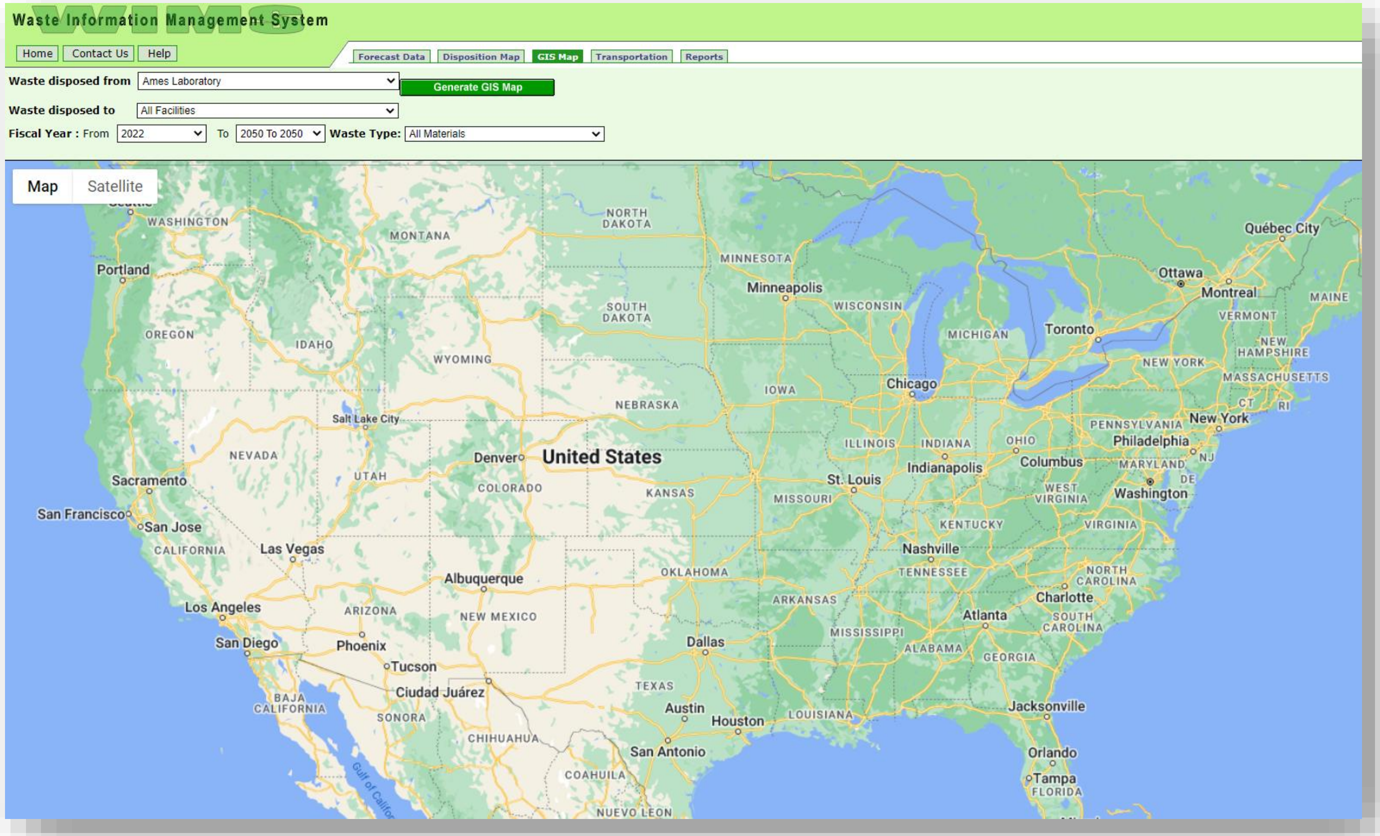
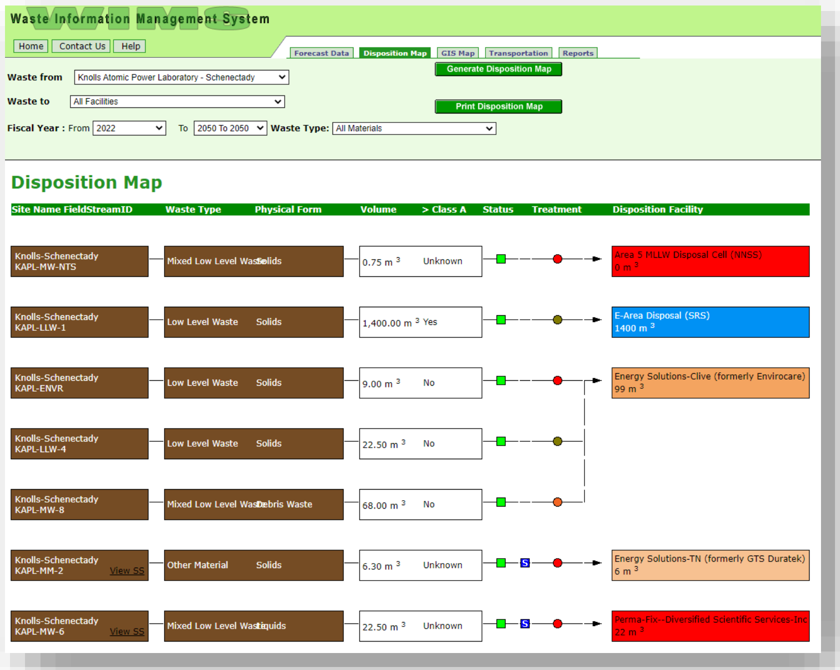
Waste Information Management System (WIMS)

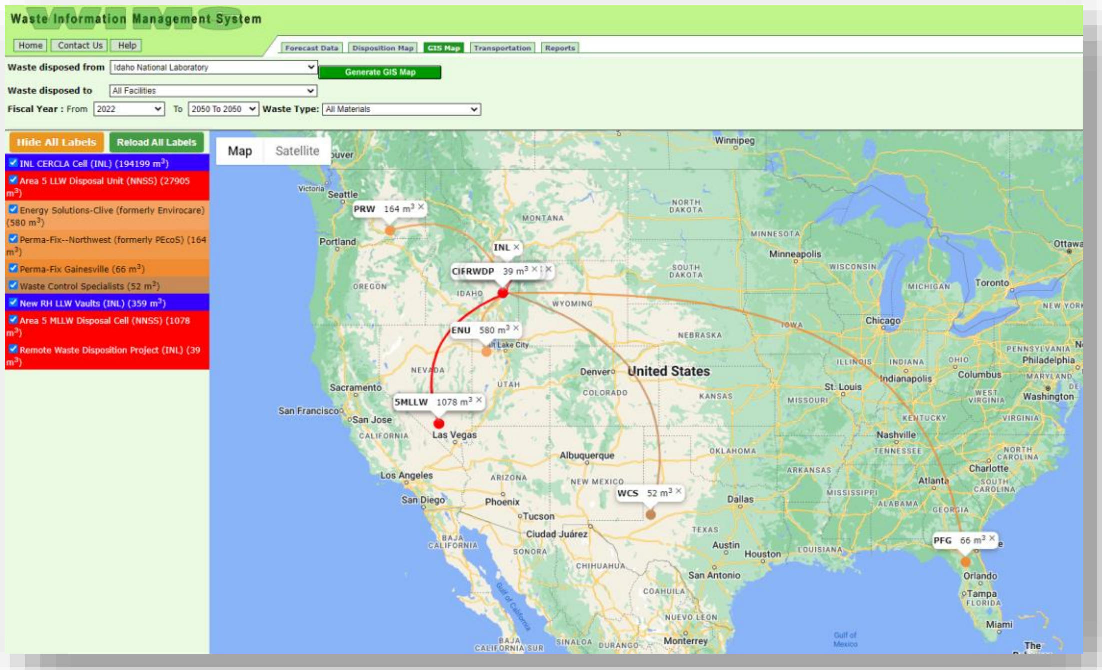
Subtask 1.1	WIMS System Administration - Database Management, Application Maintenance & Performance Tuning
Subtask 1.2	Waste Stream Annual Data Integration
Subtask 1.3	Cyber Security of WIMS Infrastructure



Waste Information Management System (WIMS)

- Easy-to-use system to visualize and understand the forecasted DOE-EM waste streams & transportation information.
- Various modules of WIMS are Forecast Data, Disposition Map, Successor Stream Map, GIS Map, Transportation, Reports and Help.
- WIMS is deployed and available at https://www.emwims.org

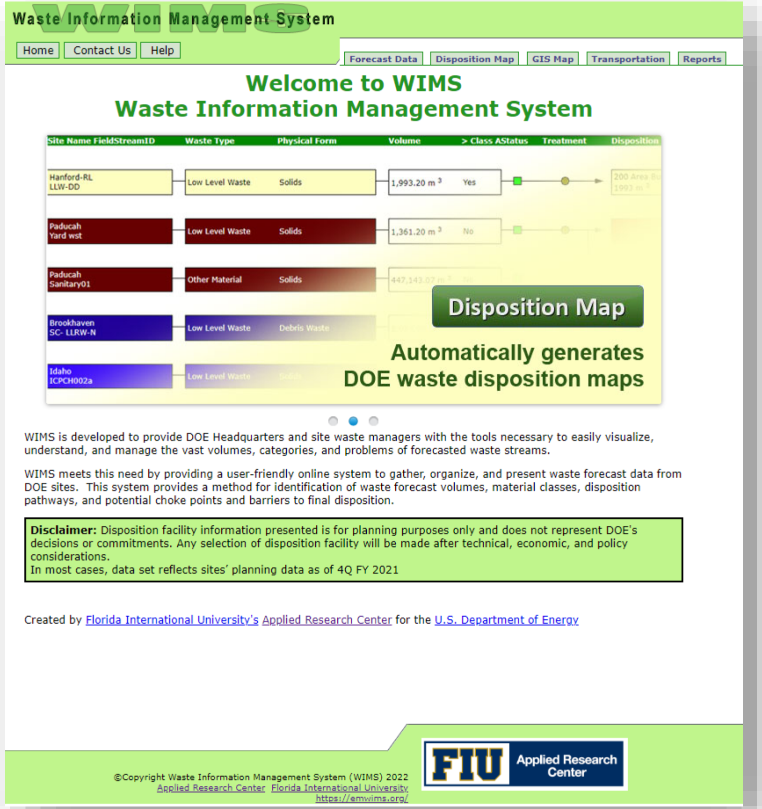


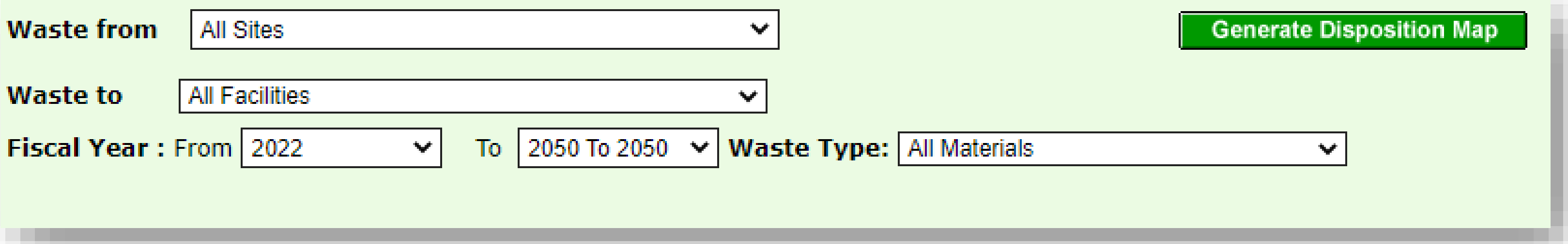


Waste Stream Annual Data Integration

Accomplishments:

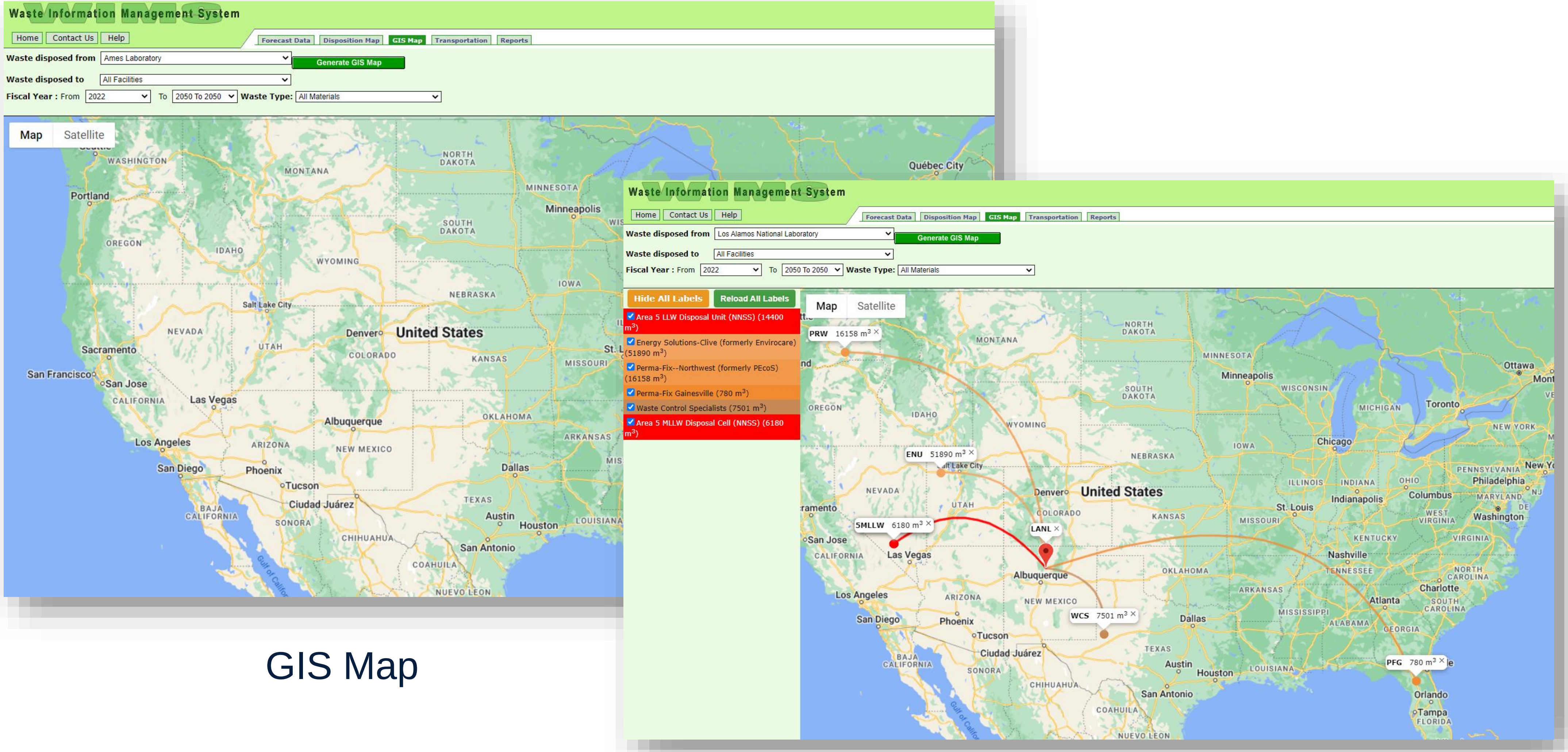
- Received and incorporated the revised waste forecast data files into the system.
- Completed integration of 2022 waste forecast and transportation data into WIMS system (Milestone 2021-P3-M3).
- Published 2022 Forecast Waste stream information on April 25, 2022.
- Presented WIMS research at 2022 Waste Management Symposia in March 2022.





Waste Stream Annual Data Integration

Accomplishments:

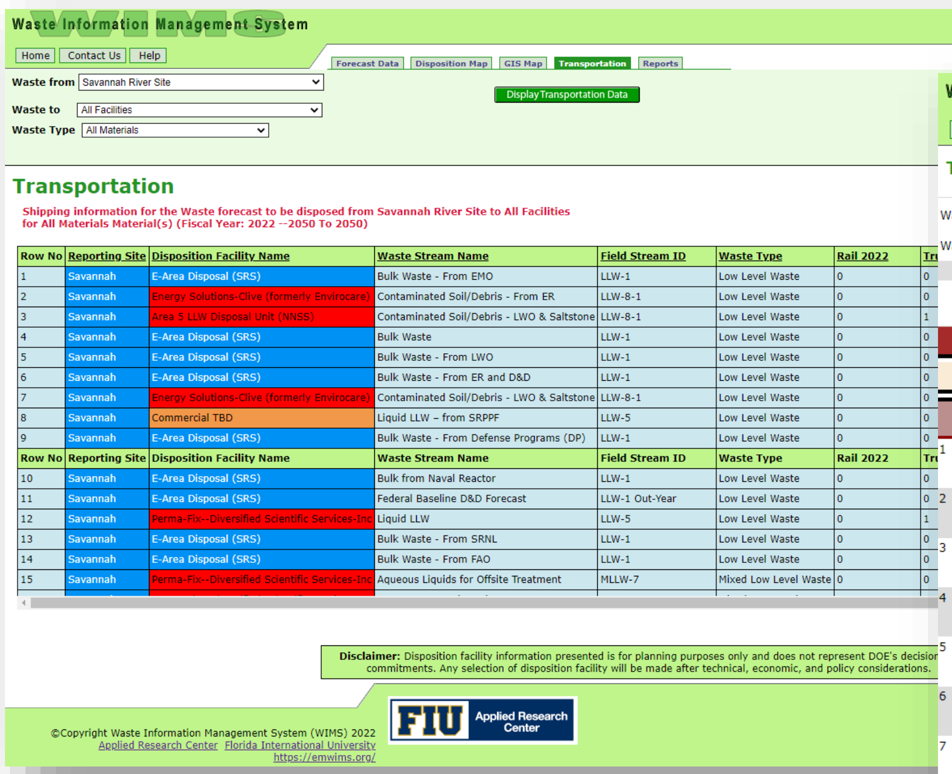


GIS Map

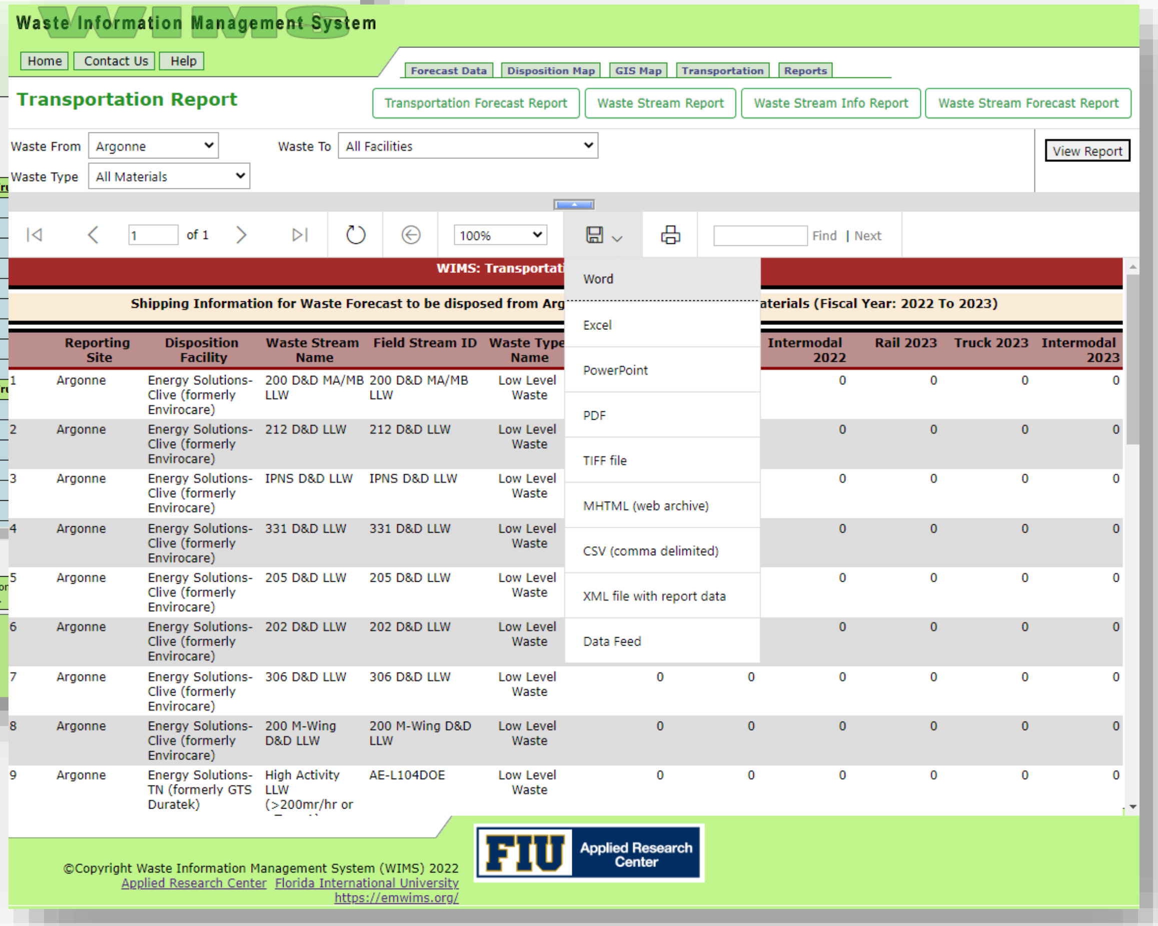
Use Google Map API for enhanced user interaction

Waste Stream Annual Data Integration

Accomplishments:



Transportation



Reports - Sample Transportation Report

The Waste Information Management System (WIMS) Development, Maintenance and New Data Integration

FIU Year 3 Projected Scope

- **Subtask 1.1: WIMS System Administration - Database Management, Application Maintenance & Performance Tuning**
  - This subtask includes the day-to-day maintenance and administration of the application and the database servers.
  - Administrator will monitor the network and server traffic and perform updates necessary to optimize the application performance.
  - FIU will provide application and database security as well as help desk support to DOE site managers, HQ managers and other users who need assistance with WIMS.
- **Subtask 1.2: Waste Stream Annual Data Integration**
  - Update WIMS modules – Forecast Data , Waste Stream and GIS map.
  - Update and publish reports.
  - Update and publish transportation module.
- **Subtask 1.3: Cyber Security of WIMS Infrastructure**
  - Provide cyber security to WIMS infrastructure, application, database server and reporting server.
  - Cybersecurity training and support of DOE Fellows while working with pen testing & forensics tools used with WIMS system.

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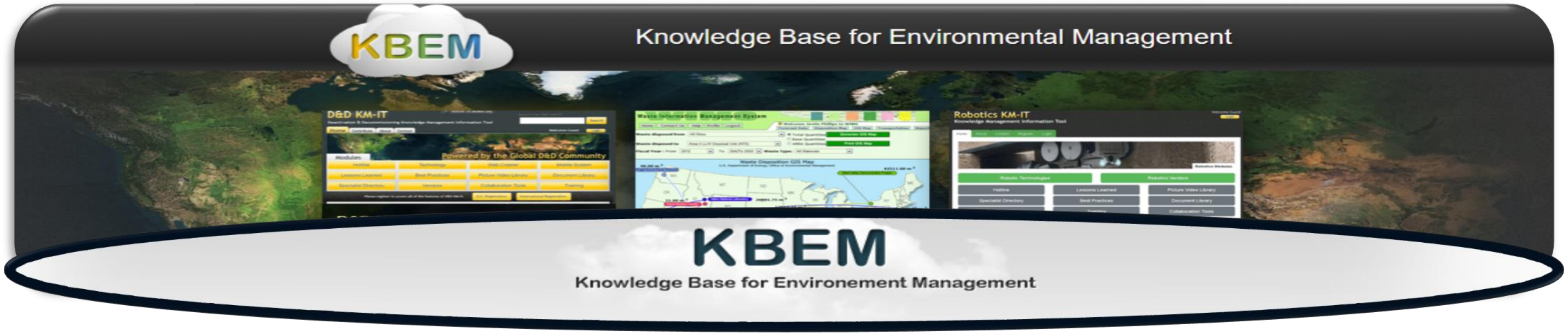
Task 3

D&D Knowledge Management Information Tool (KM-IT)

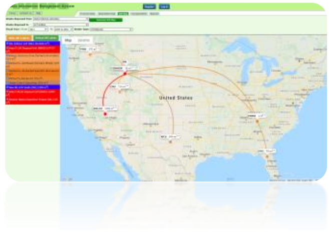
Task 3: D&D Knowledge Management Information Tool (KM-IT)

Subtask 3.4	Content Management
Subtask 3.5	Marketing and Outreach
Subtask 3.6	D&D KM-IT System Administration
Subtask 3.7	Cyber Security of D&D KM-IT Infrastructure
Subtask 3.8	KM-IT Tech Talks

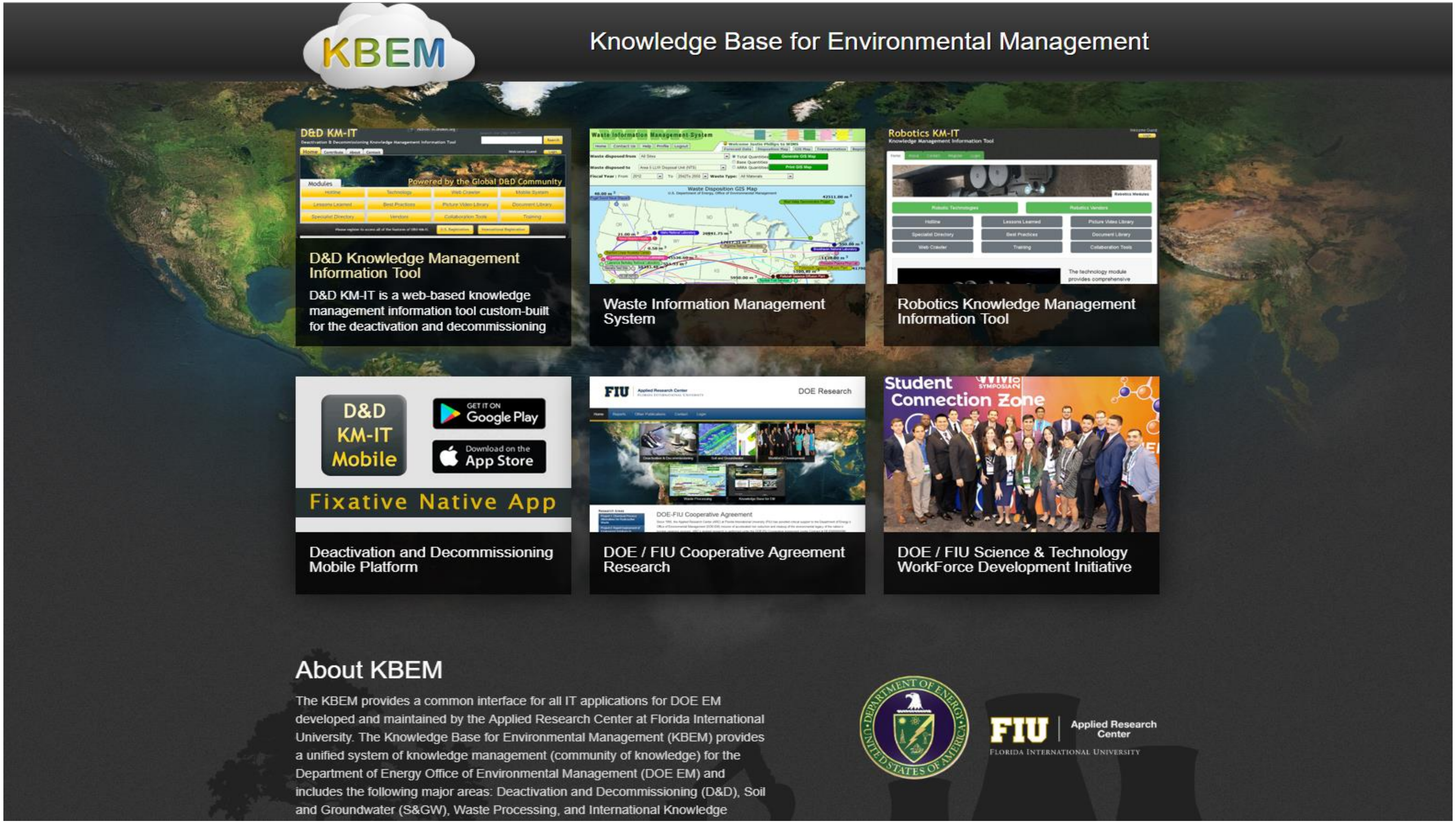
Knowledge Base for Environmental Management



DND KM-IT	WIMS	DOE FELLOWS	DOE RESEARCH	Robotics KM-IT
dndkm.org	emwims.org	fellows.fiu.edu	doeresearch.fiu.edu	rkmit.org


Knowledge Base for Environmental Management



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Content Management

Accomplishments:

- Published D&D technologies, vendors, D&D technologies, lessons learned, best practices, D&D news, conferences and other content to KM-IT.
- Performed QA/QC of existing content in the system with assistance of DOE Fellows.
- 107 technologies were published on this platform in this fiscal year, bringing the total technologies published to 1,544.
- 655 technologies published in the last 3 years

Portable Fume Extractor

Robotic Welders

Anti-Contamination “Blu” Suit

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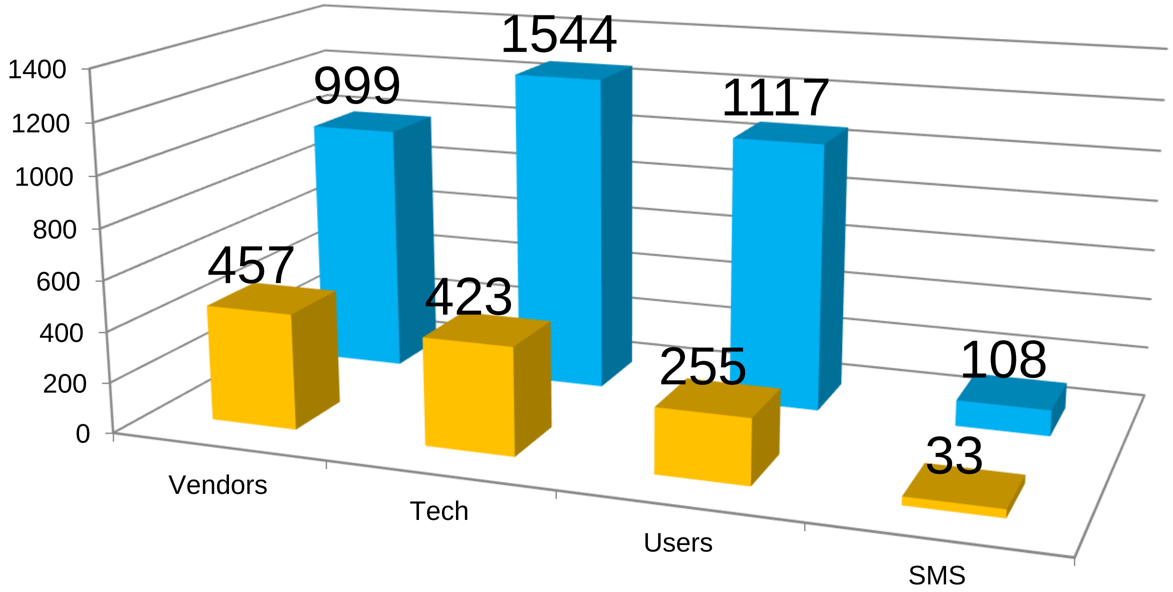
Content Management

Description and Accomplishments:

- D&D KM-IT web analytics to track usage metrics
- 1,544 D&D technologies
- 1,117 registered users
- 999 D&D vendors
- 108 subject matter specialists

Yellow – March, 2012 Blue – August, 2022

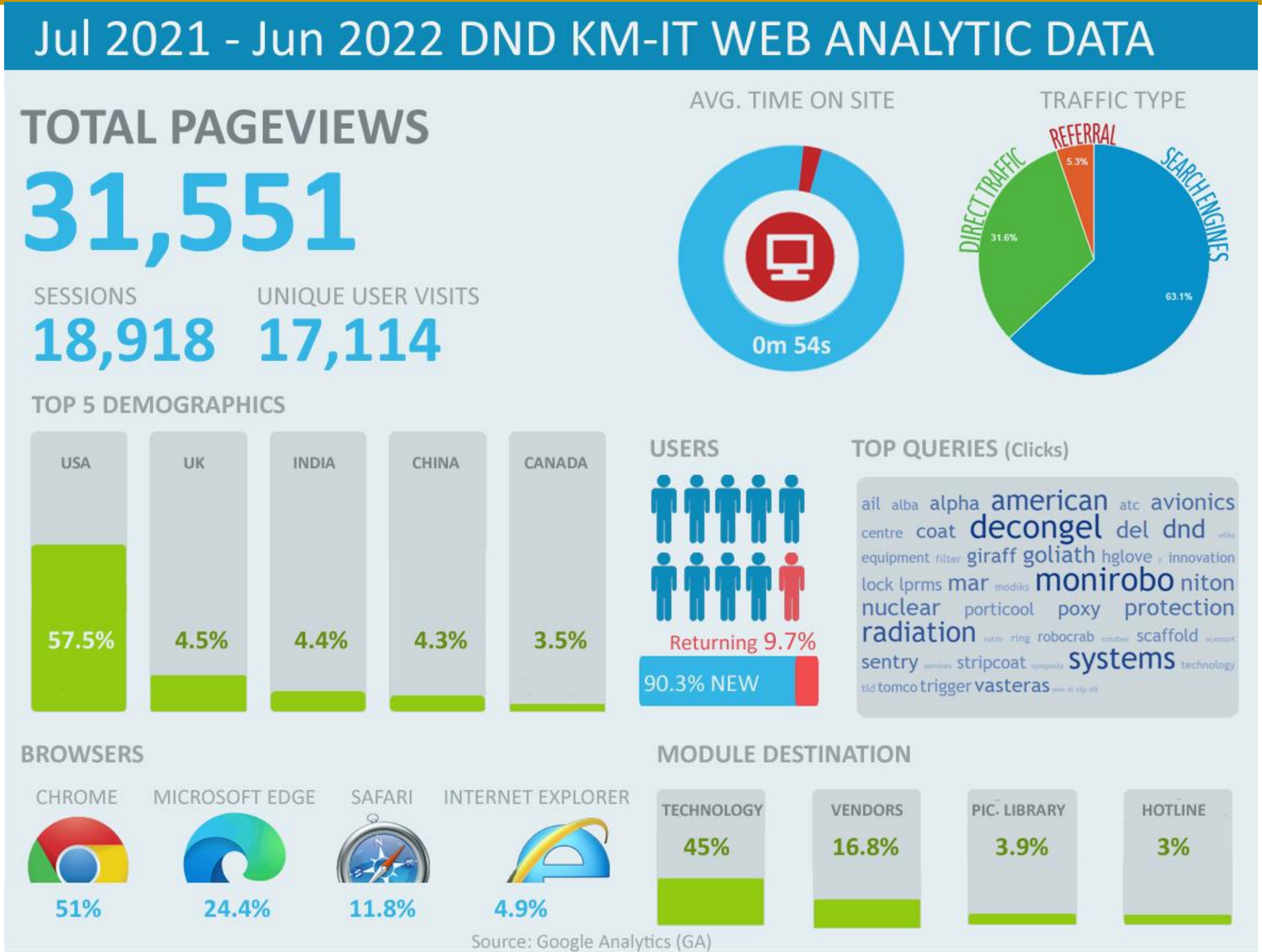


Growth from March 2012 to Aug 2022

<u>Fully searchable resources – Original sources no longer available</u>

- 169 ALARA Center reports archived (Hanford and SRS)
- 231 Innovative Technology Summary Reports archived

Subtask 3.4: Content Management



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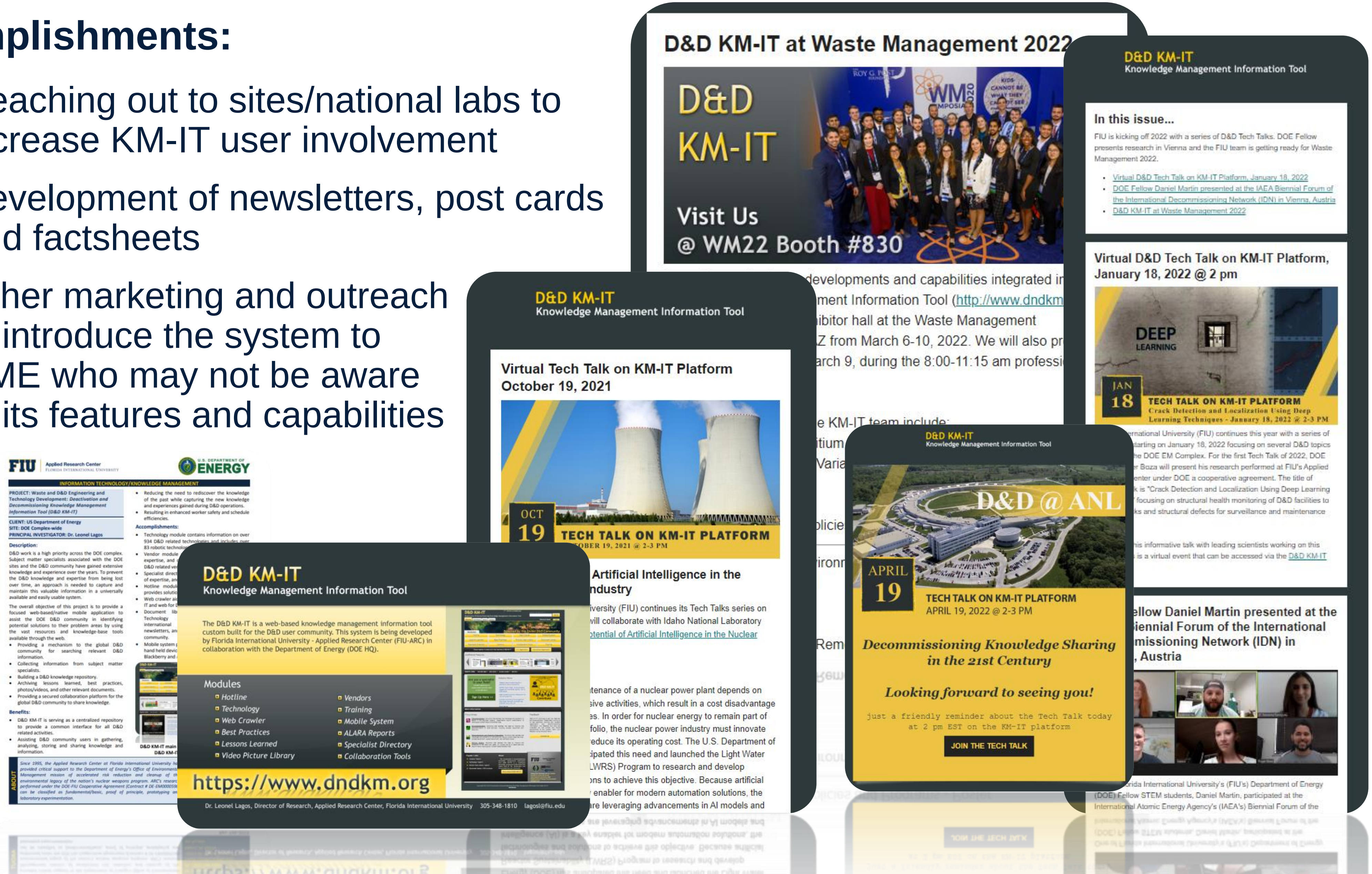
Marketing and Outreach

Accomplishments:

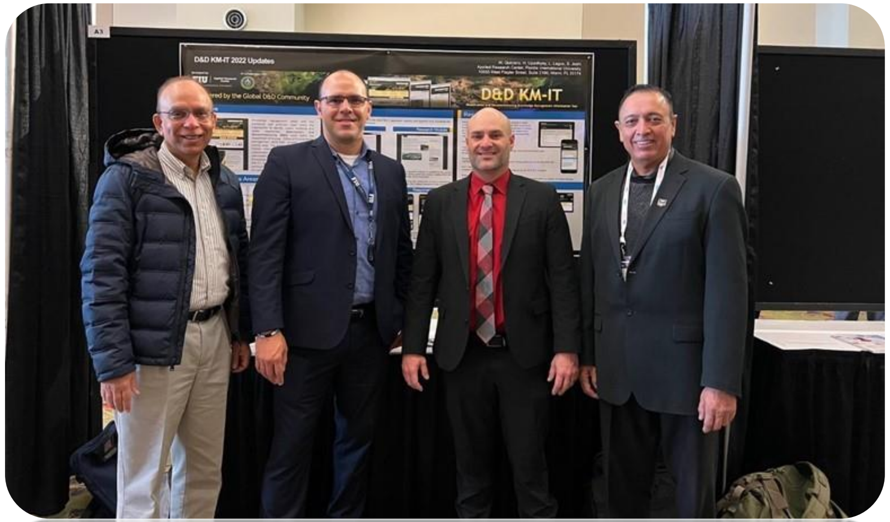
- Reaching out to sites/national labs to increase KM-IT user involvement
- Development of newsletters, post cards and factsheets
- Other marketing and outreach to introduce the system to SME who may not be aware of its features and capabilities



Subtask 3.5: Marketing and Outreach

Accomplishments:

- Participation at workshops and conferences such as the Waste Management Symposia
  - FIU ARC Booth
  - Presented AI application to D&D problem set - **Best Oral Presentation Award**
  - Presented KM-IT poster at WM2022
  - Presented WIMS poster at WM2022



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KM-IT Tech Talks

Accomplishments:

- Conducted D&D-related Tech Talk every quarter on the D&D KM-IT platform.
- Collaborated with National Laboratories and/or DOE sites to identify and present technical topics of interest to the community.
- Tech Talks are conducted virtually using an online meeting platform that can be accessed via KM-IT
- Promoted Tech Talks via newsletters, website, emails and flyers developed by FIU.
- Conducted 4 Tech Talks:
    - October 19, 2021
      The Potential of Artificial Intelligence in the Nuclear Power Industry
    - January 18, 2022
      Crack Detection and Localization Using Deep Learning Technique
    - April 19, 2022
      Decommissioning Knowledge Sharing in the 21st Century
    - July 19, 2022
      Understanding Decontamination (and a dozen other lessons)

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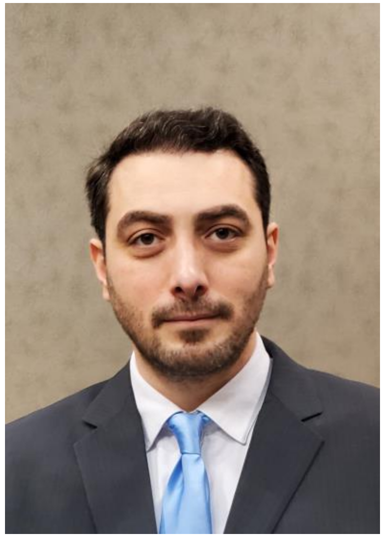
KM-IT Tech Talks

Accomplishments:

October 19, 2021
The Potential of Artificial Intelligence in the Nuclear Power Industry

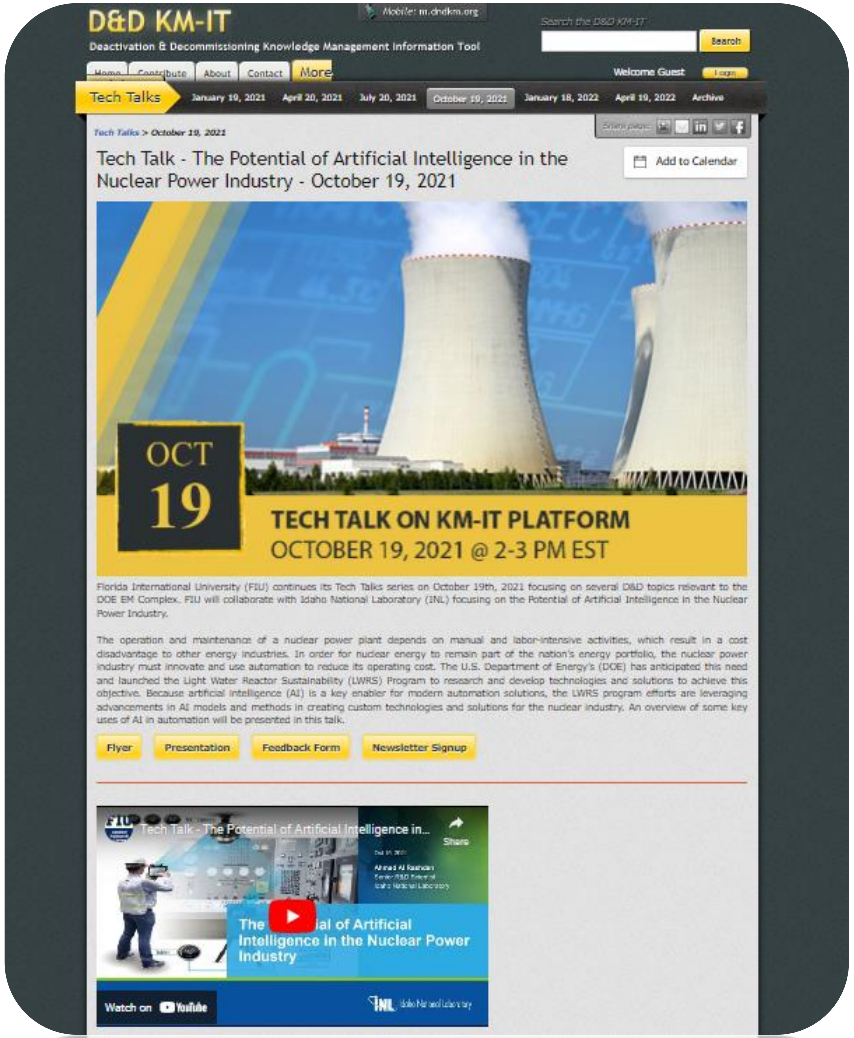
Topic:
Potential of artificial intelligence in the nuclear power industry

Collaborator:
Idaho National Laboratory (INL)



Speaker:
Dr. Ahmad Rashdan

Senior research and development scientist at Idaho National Laboratory (INL)



KM-IT Tech Talks

Accomplishments:

January 18, 2022
Crack Detection and Localization Using Deep Learning Techniques

Topic:
Using deep learning techniques to detect infrastructure cracks at DOE facilities

Collaborator:
FIU Research

Speaker:
Roger Boza

DOE Fellow pursuing a Ph.D. in Computer Science with a focus on machine learning (M.L.), artificial intelligence (A.I.), and deep learning (D.L.) techniques

Accomplishments:

April 19, 2022
Decommissioning Knowledge Sharing in the 21st Century

Topic:
Decommissioning activities and techniques, lessons learned and best practices

Collaborator:
Argonne National Laboratory

Speaker:
Lawrence (Larry) Boing

Senior Staff
Facility Decommissioning SME and D&D Experiences KM Training Director

KM-IT Tech Talks

Accomplishments:

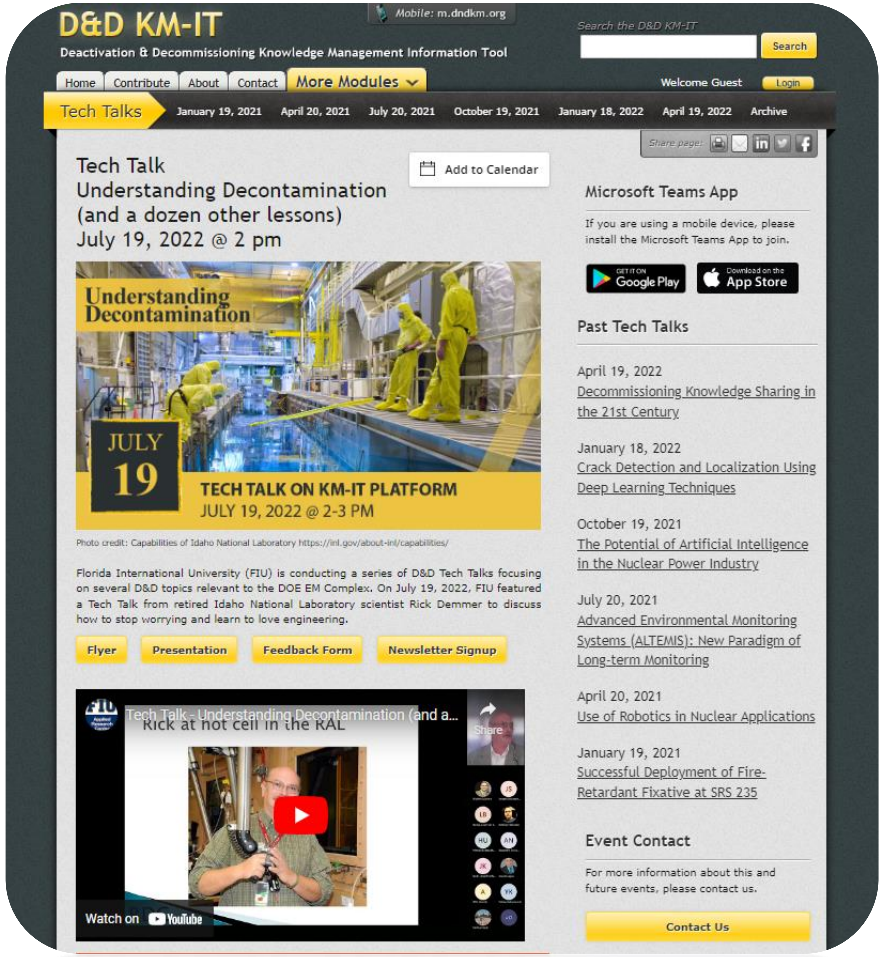
July 19, 2022
Understanding Decontamination (and a dozen other lessons)

Topic:
Discussing how to stop worrying and learn to love engineering to get the work done

Collaborator:
Idaho National Laboratory (INL)

Speaker:
Rick Demmer, Ph.D

Senior Staff
Retired scientist, project manager and distinguished scientist from the Idaho National Laboratory
(39 years tenure at the INL)



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KM-IT Tech Talks

Next Tech Talk:

October 18, 2022
University R&D and Deployment of Robotics Systems at DOE Facilities

Topic:
Recent robotic technologies deployment by FIU at DOE Facilities

Collaborator:
FIU Robotics Research Team

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D&D KNOWLEDGE MANAGEMENT INFORMATION TOOL (KM-IT) (HQ, SRNL, INL, ANL)

FIU Year 3 Projected Scope

- **Subtask 3.4: Content Management**
  - Publishing D&D technologies, vendors, D&D technologies, lessons learned, best practices, D&D news, conferences and other content to KM-IT
  - Perform QA/QC of existing content in the system with assistance of DOE Fellows
- **Subtask 3.5: Marketing and Outreach**
  - Reaching out to sites/national labs to increase KM-IT user involvement
  - Participation at workshops and conferences such as Waste Management and engagement with other agencies such as the IAEA.
  - Introduce the system to SME who may not be aware of its features and capabilities
  - Development of newsletters, post cards, factsheets and other print material to promote KM-IT
- **Subtask 3.6: D&D KM-IT System Administration**
  - D&D KM-IT System Administration is an ongoing task which involves day-to-day administration of servers that house the KM-IT databases and web applications.
  - This task includes updating patches and OS fixes, updating antivirus engines and definitions, updating drivers and assuring that the network (firewall, routers and switches) is working properly.

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D&D KNOWLEDGE MANAGEMENT INFORMATION TOOL (KM-IT) (HQ, SRNL, INL, ANL)

FIU Year 3 Projected Scope

- **Subtask 3.7: Cyber Security of D&D KM-IT Infrastructure**
  - Cyber Security of D&D KM-IT Infrastructure involves securing the network not only by system administration tasks mentioned above, but also by conducting routine cyber security tasks to test the network's vulnerability.
  - This involves coordination between the FIU security team and DOE Fellows who learn cybersecurity skills while assisting staff do penetration testing and other tasks to test the overall security of the system at the application, database and infrastructure levels.
- **Subtask 3.8: KM-IT Tech Talks**
  - Conduct D&D related Tech Talk every quarter on the D&D KM-IT platform.
  - Collaborate with National Laboratories and/or DOE sites to identify and present technical topics of interest to the community.
  - Tech Talks will be performed virtually using an online meeting platform (KM-IT)
  - Promote Tech Talks via newsletters, website, emails and flyers developed by FIU.

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Task 6

AI for EM Problem Set (D&D) – Structural Health Monitoring of D&D Facility to Identify Cracks and Structural Defects for Surveillance and Maintenance (SRNL)

Task 6 : AI for EM Problem Set (D&D): Structural Health Monitoring of D&D Facility to Identify Cracks and Structural Defects for Surveillance and Maintenance (SRNL)

Subtask 6.5	Design & Development of Machine Learning and Deep Learning Models to Identify and Locate Cracks in D&D Mockup Facility
Subtask 6.6	Design & Development of a Mobile Application to Deploy Machine Learning and Deep Learning Models on the iOS Devices at SRS
Subtask 6.7	Research and Prototype Deployment of a Web Service API framework for AI Deep Learning Model

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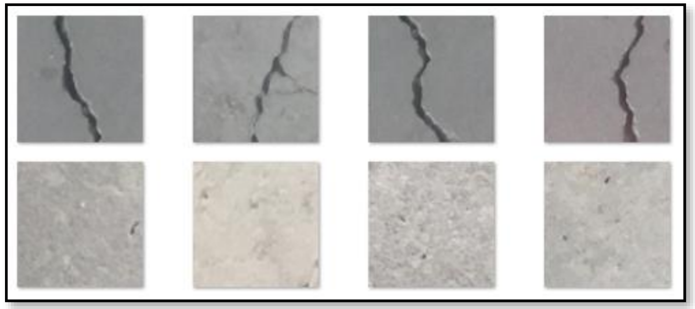
Design & Development of Machine Learning and Deep Learning Models to Identify and Locate Cracks in D&D Mockup Facility

FIU Year 2 Research Highlights:

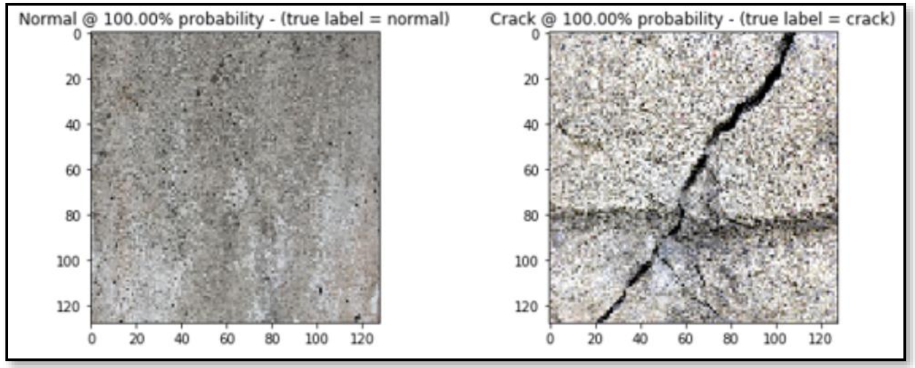
- **Developing and training new classification models.**
  - Trained and tested 6 Convolutional Neural Networks (CNN) for classifying images.
  - The training dataset was composed of 20,000 images with cracks and 20,000 images without cracks.
  - All models achieved over 98% validation accuracy.



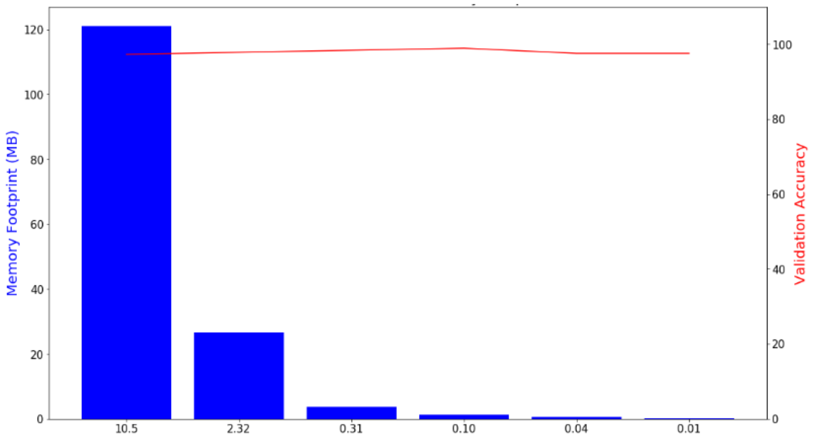
Training data sample

Model name	Total number of convolutional layers	Total Parameters (Millions)	Memory Footprint (MB)	Validation accuracy
M1	4	0.01	0.23	98.1%
M2	4	0.04	0.55	98.2%
M3	3	0.10	1.26	98.4%
M4	6	0.31	3.64	98.4%
M5	6	2.32	26.6	98.8%
M6	6	10.5	121	99.1%
VGG16	16	15	197	99.4%

Model memory footprint and validation accuracy



Prediction results on sample images



Physical memory and performance analysis

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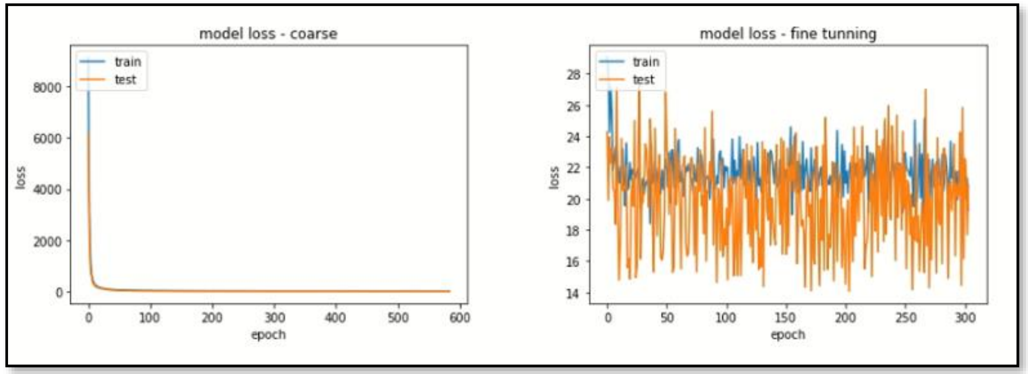
Design & Development of Machine Learning and Deep Learning Models to Identify and Locate Cracks in D&D Mockup Facility

FIU Year 2 Research Highlights:

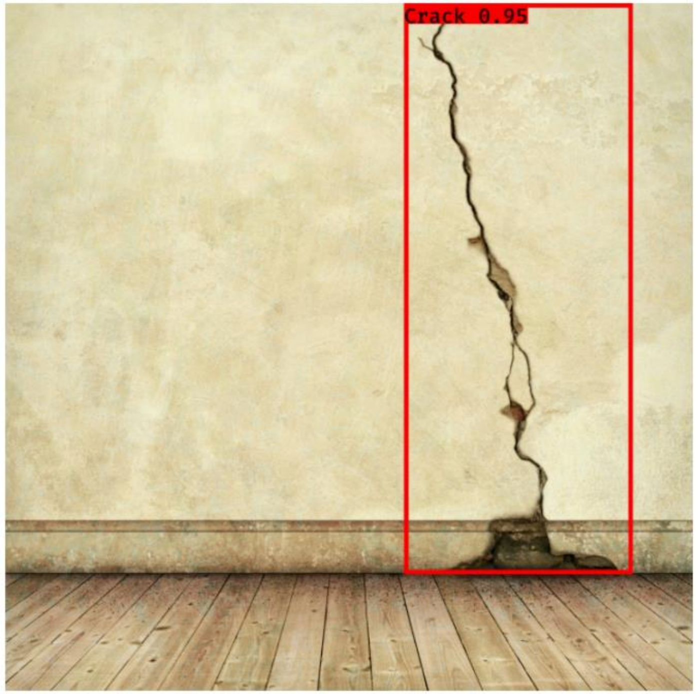
- **Object detection with You Only Look Once (YOLOv3)**
  - Better YOLOv3 crack detection model with tighter bounding boxes and higher confidence scores.
  - Used Keras callback functions to stop the training early when the loss function did not improve over time.
  - Reduction of learning rate on plateau during fine tuning.

```
Epoch 577/1000
5/5 [==============================] - 4s 801ms/step - loss: 25.7063 - val_loss: 23.5676
Epoch 578/1000
5/5 [==============================] - 4s 847ms/step - loss: 28.8526 - val_loss: 27.2604
Epoch 579/1000
5/5 [==============================] - 4s 808ms/step - loss: 27.8816 - val_loss: 25.3630
Epoch 580/1000
5/5 [==============================] - 4s 828ms/step - loss: 31.7066 - val_loss: 20.1554
Epoch 581/1000
5/5 [==============================] - 4s 809ms/step - loss: 29.9588 - val_loss: 28.0598
Epoch 582/1000
5/5 [==============================] - 4s 826ms/step - loss: 27.6605 - val_loss: 21.4318
Epoch 583/1000
5/5 [==============================] - 4s 824ms/step - loss: 28.2139 - val_loss: 21.6117
Epoch 584/1000
5/5 [==============================] - 4s 819ms/step - loss: 26.9793 - val_loss: 22.5110
Epoch 00584: early stopping
```

Early stopping during model training



Model loss value during coarse training and fine tuning



Crack object detection results

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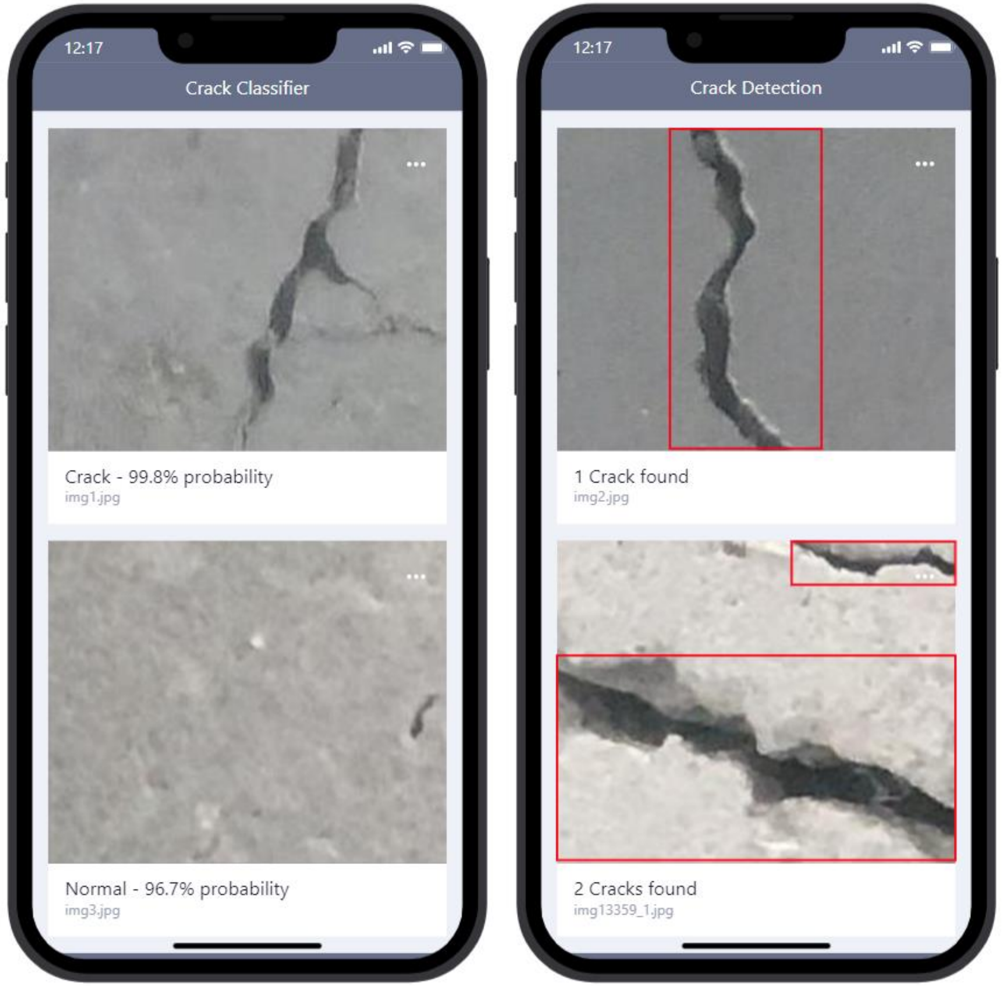
Design & Development of a Mobile Application to Deploy Machine Learning and Deep Learning Models on the iOS Devices at SRS

FIU Year 2 Research Highlights:

- **Graphical user interface for mobile device**
  - Mobile application can classify images as either crack or normal.
    - Using the trained CNN classifiers.
    - Using state-of-the-art models:
      - VGG16
      - RESNET50
      - MOBILENET
  - Mobile application can detect and locate cracks in images.
    - As well as facemask (custom trained model)
    - The 1,000 common objects in the COCO dataset.



Crack classification (left) and crack object detection (right)

Task 6 : AI for EM Problem Set (D&D): Structural Health Monitoring of D&D Facility to Identify Cracks and Structural Defects for Surveillance and Maintenance (SRNL)

Task is Completed:

- **Project 3 Task 6 Deliverable**
  - 2021-P3-D7 (9/9/2022)
    - Design & Development of Machine Learning and Deep Learning Models to Identify and Locate Cracks in D&D Mockup Facility Deployed on Mobile App Supported by Web API

COMPLETED!

- **Work done for Task 6 will be applied to Task 9**

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Task 9

AI for EM Problem Set (Waste Processing):

Nuclear Waste Identification and Classification using Deep learning (SRNL) (NEW)

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Task 9 - AI for EM Problem Set (Waste Processing) (SRNL)

FIU Year 3 Projected Scope

- **Subtask 9.1: Algorithm & Model Development to Identify and Classify Nuclear Wastes**
  - Research state-of-the-art Artificial Intelligence (AL) algorithms like Machine Learning (ML) and Deep Learning (DL) to segregate LLW.
  - Nuclear Waste Identification and Classification of LLW using algorithms and models.
- **Subtask 9.2: Transition Previously Trained Deep Learning Models to the Advance Automated Machine Learning (AAML) System**
  - The state-of-the-art ML/DL models trained and optimized for image classification and object detection of LLW will be published to the Advance Automated Machine Learning (AAML) platform.

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Task 7

AI for EM Problem Set (Soil & GW):

Exploratory Data Analysis and Machine Learning Model for Hexavalent Chromium [Cr (VI)] Concentration in 100-H Area (PNNL)

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Task 7: AI for EM Problem Set (Soil & GW): Exploratory Data Analysis and Machine Learning Model for Hexavalent Chromium [Cr (VI)] Concentration in 100-H Area

Subtask 7.2	Data Pre-processing and Exploratory Data Analysis to Evaluate the Chromium Concentration in the Samples
Subtask 7.3	Groundwater and Surface Water Spatiotemporal Relationship Identification

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Data Pre-processing and Exploratory Data Analysis to Evaluate the Chromium Concentration in the Samples

- Subsurface Chromium transport temporal and spatial relationships identification using Artificial Intelligence and Machine Learning.
- Data pre-processing to evaluate and find methods to understand the chromium concentration in groundwater and aquifer tube samples.
- Perform exploratory data analysis using state-of-the-art statistical methods.
- Develop Artificial Intelligence and Machine Learning algorithm for spatiotemporal relationship exploration.

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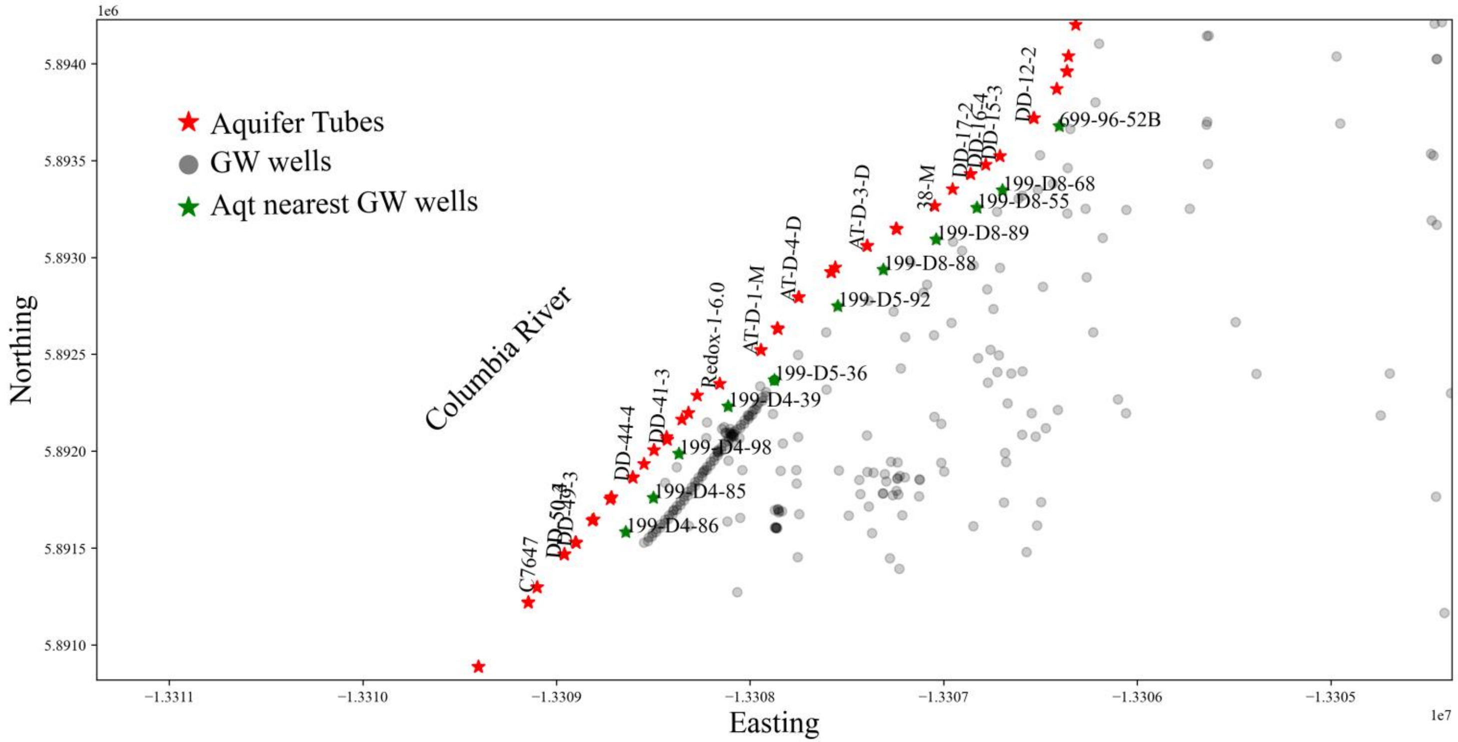
Subtask 7.2: Data Pre-processing and Exploratory Data Analysis to Evaluate the Chromium Concentration in the Samples

FIU Year 2 Research Highlights:

Data Pre-Processing for Aquifer Tubes:

- A data filter algorithm was designed for 100-HR-D area data, and 15 aquifer tubes were obtained from the algorithm for further processing which are denoted by the red star in the plot.
- Shoreline groundwater well identification feature was included in the algorithm to find and use groundwater wells as a proxy or target in addition to the aquifer tubes based on data density.

Adjacent Groundwater wells of Aquifer tubes



Data pre-processing and exploratory data analysis to evaluate the chromium concentration in the samples

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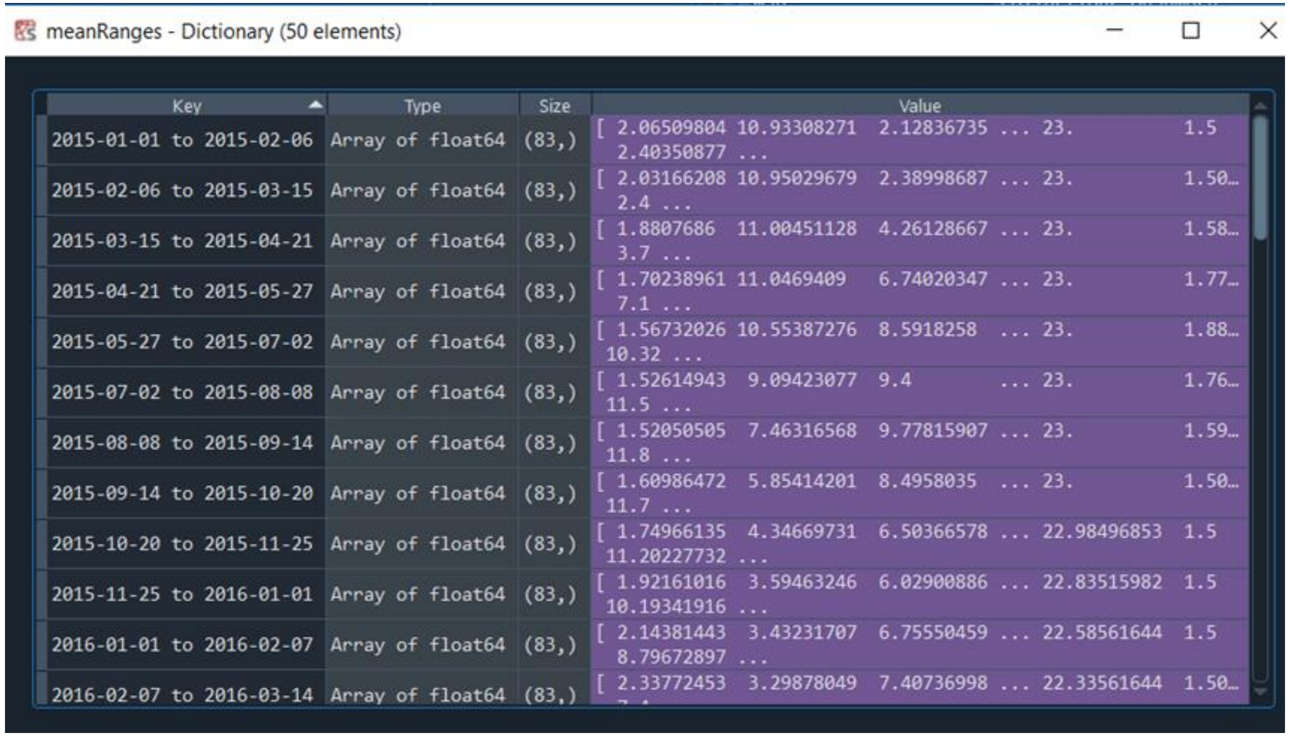
FIU Year 2 Research Highlights:

Further Data preprocessing:

- Grouping of chromium concentration data of each of the 83 wells was done into periods of time.
- The 1,826 dates ranging from 2015 till 2019 were split into 50 periods with each period containing the chromium concentration mean values for further analysis in later machine learning modeling.
- Each period contained mean concentration values for the 83 wells for a range of 1 month, 6 days.


meanRanges - Dictionary (50 elements)

Key	Type	Size	Value
2015-01-01 to 2015-02-06	Array of float64	(83,)	[2.06509804 10.93308271 2.12836735 ... 23. 1.5 2.40350877 ...
2015-02-06 to 2015-03-15	Array of float64	(83,)	[2.03166208 10.95029679 2.38998687 ... 23. 1.50… 2.4 ...
2015-03-15 to 2015-04-21	Array of float64	(83,)	[1.8807686 11.00451128 4.26128667 ... 23. 1.58… 3.7 ...
2015-04-21 to 2015-05-27	Array of float64	(83,)	[1.70238961 11.0469409 6.74020347 ... 23. 1.77… 7.1 ...
2015-05-27 to 2015-07-02	Array of float64	(83,)	[1.56732026 10.55387276 8.5918258 ... 23. 1.88… 10.32 ...
2015-07-02 to 2015-08-08	Array of float64	(83,)	[1.52614943 9.09423077 9.4 ... 23. 1.76… 11.5 ...
2015-08-08 to 2015-09-14	Array of float64	(83,)	[1.52050505 7.46316568 9.77815907 ... 23. 1.59… 11.8 ...
2015-09-14 to 2015-10-20	Array of float64	(83,)	[1.60986472 5.85414201 8.4958035 ... 23. 1.50… 11.7 ...
2015-10-20 to 2015-11-25	Array of float64	(83,)	[1.74966135 4.34669731 6.50366578 ... 22.98496853 1.5 11.20227732 ...
2015-11-25 to 2016-01-01	Array of float64	(83,)	[1.92161016 3.59463246 6.02900886 ... 22.83515982 1.5 10.19341916 ...
2016-01-01 to 2016-02-07	Array of float64	(83,)	[2.14381443 3.43231707 6.75550459 ... 22.58561644 1.5 8.79672897 ...
2016-02-07 to 2016-03-14	Array of float64	(83,)	[2.33772453 3.29878049 7.40736998 ... 22.33561644 1.50…

- The Key column contains the 50 date ranges or periods.
- The Value column contains the mean concentration values for all 83 groundwater wells identified.

Groundwater and Surface Water Spatiotemporal Relationship Identification

FIU Year 2 Research Highlights:

Spatial and temporal information fusion:

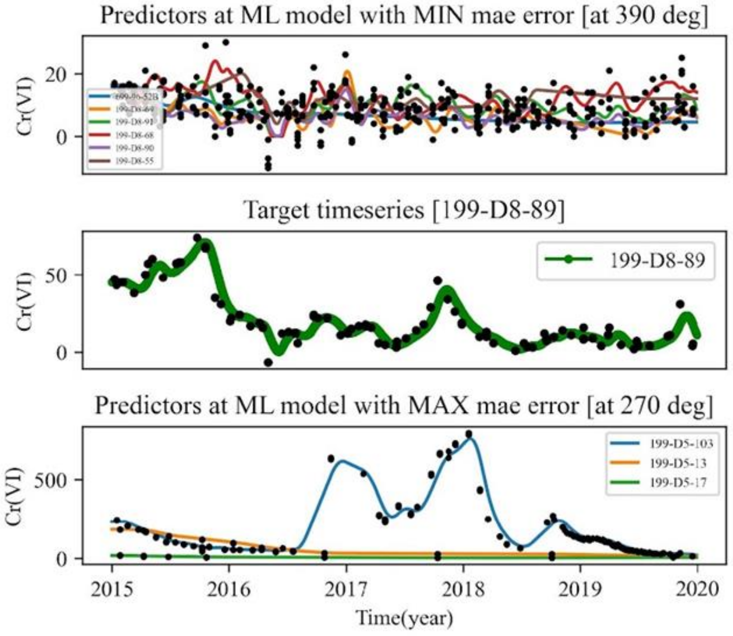
- For each of the target wells in the ML model, angles ranging from 225 to 390 degrees and radius up to 1500m, were explored for the ML models’ performance at directions and distances.
- Support Vector Machine, Random Forest, K-nearest Neighbor and Regression algorithms were applied for ML model development with each proxy groundwater well as the target, and with each of the aquifer tubes as the target.

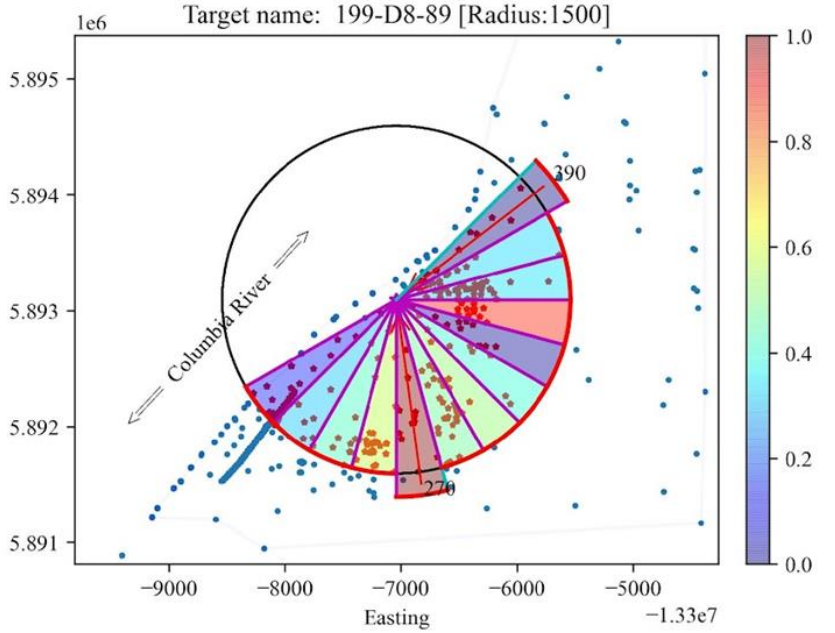
List of wells

```
-----------
199-D8-89
Radius:1500

Predictors at ML
model with
MIN mae error
[at 390 deg]
['699-96-52B',
'199-D8-69',
'199-D8-91',
'199-D8-68',
'199-D8-90',
'199-D8-55']

Predictors at ML
model with
MAX mae error
[at 270 deg]
['199-D5-103',
'199-D5-13',
'199-D5-17']
```

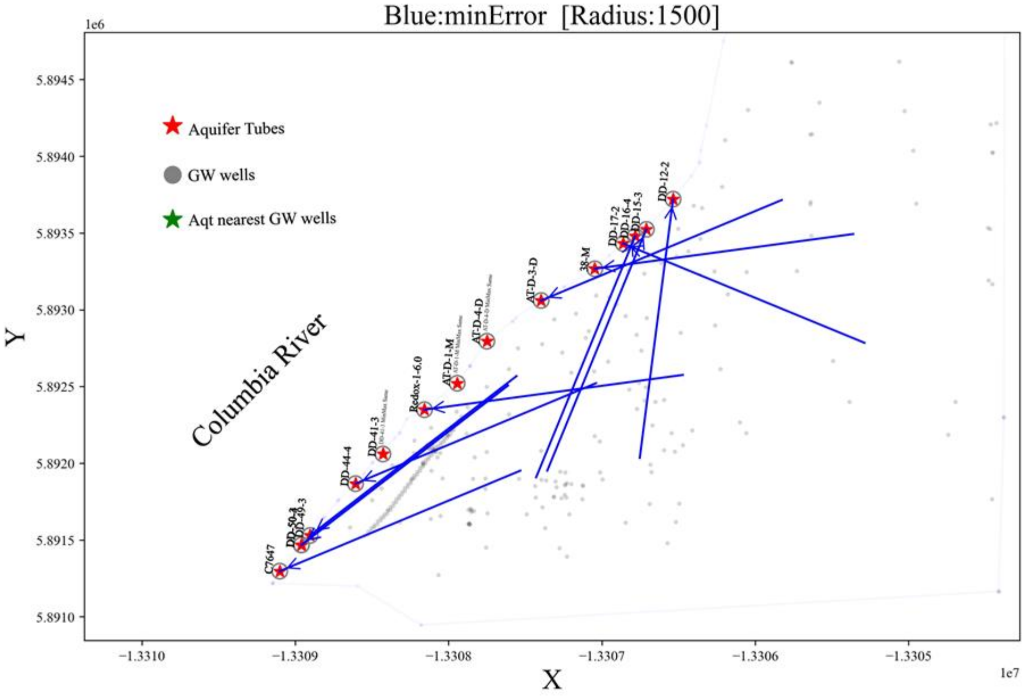




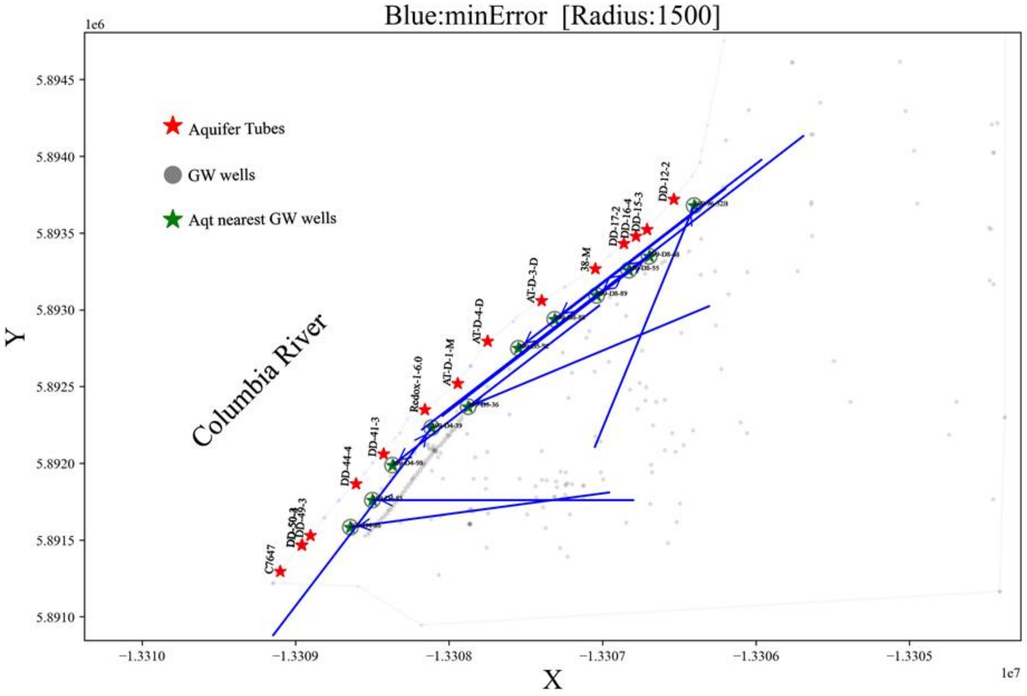
Groundwater and Surface Water Spatiotemporal Relationship Identification

FIU Year 2 Research Highlights:

The Outcome Of The Regression Analysis As Spatiotemporal Relation



The blue lines indicate with minimum error how similar the Hexavalent Chromium concentration values are for the aquifer tube wells in that direction.



The blue lines indicate with minimum error how similar the Hexavalent Chromium concentration values are for the closest groundwater wells in that direction.

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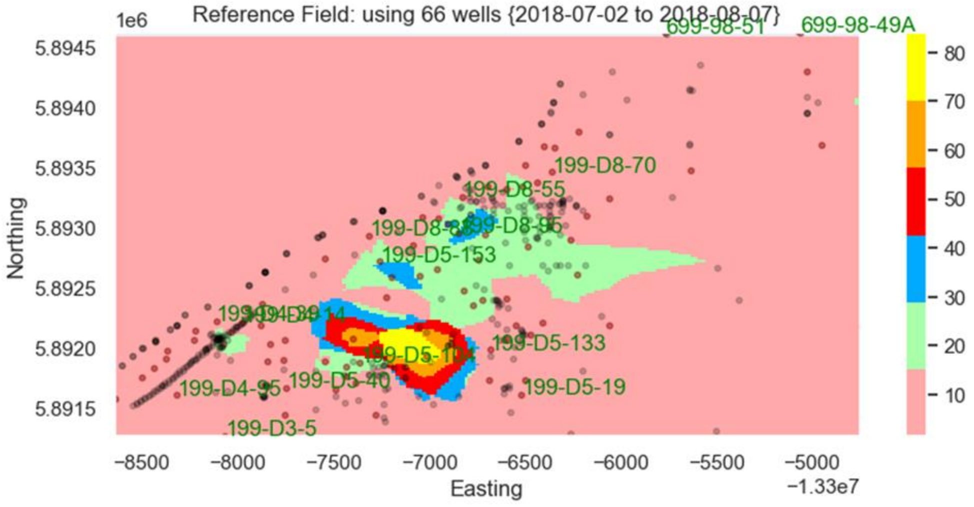
Groundwater and Surface Water Spatiotemporal Relationship Identification

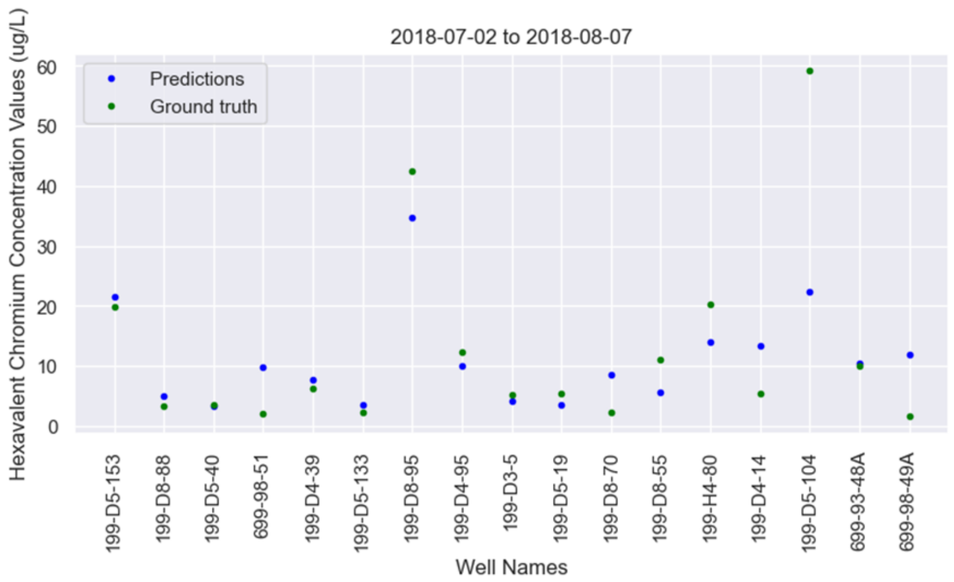
FIU Year 2 Research Highlights:

Spatial and Temporal Prediction Modeling

- The main objective for Spatial Prediction modeling was, given the location of within 100-HR-D, predict the chromium concentration level. Input to the ML model was location data and output was concentration data for the location.
- The main benefit of these ML models is that for the entire 100-HR-D area, even a location with no monitoring well could have its concentration level predicted spatiotemporally, thus giving us a larger overall picture into spatiotemporal relationships in the area.



Spatial Prediction on entire field



Spatial Prediction Accuracy for known location

FIU Year 3 Projected Scope

- **Subtask 7.4: Algorithm development for spatiotemporal relationship identification**

  The research on the spatiotemporal relationship exploration will be extended with machine learning and deep learning algorithms such as Naïve Bayes, K-means, Recurrent Neural Network – Long Short-Term Memory (RNN-LSTM).

- **Subtask 7.5: Publishing AI/ML models on AAML System**

  As part of the spatiotemporal relationship identification, algorithms were developed for data pre-processing, exploratory data analysis, and direction-wise important groundwater wells identification for surface water Cr(VI) predictive AI/ML models. FIU will be publishing these models on an Advanced Automated Machine Learning (AAML) system, which is a web-based system deployed in FIU infrastructure where users can view the models and prediction results.

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Task 8

AI for EM Problem Set (Soil and Groundwater) – AI System interface for sensor data ingestion and descriptive visual and data analytics (LBNL, SRNL)

Task 8: AI for EM Problem Set (Soil & GW):Data analysis and visualization of sensor data from the wells at the SRS F-Area using machine learning

Subtask 8.1	Exploratory Data Analysis
Subtask 8.2	Identify the Master/Proxy Variables
Subtask 8.3	Machine Learning Model Development & Optimization for Sensor Placement in Groundwater Wells

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Task 8:AI for EM Problem Set (Soil and Groundwater) – AI System interface for sensor data ingestion and descriptive visual and data analytics (LBNL, SRNL)

- Develop machine learning tools to automate the monitoring and forecasting of contaminant transport dynamics at the Savannah River Site (SRS) F-Area to support DOE-EM's goal for long time monitoring of contaminated groundwater sites.
- Develop data exploration tools for understanding the spatial and temporal distribution of the F-Area dataset.
- Develop a spatial interpolation approach for estimating a plume.
- Examine proxy variables at the site.
- Development of the AI/ML based system to perform predictive analytics.

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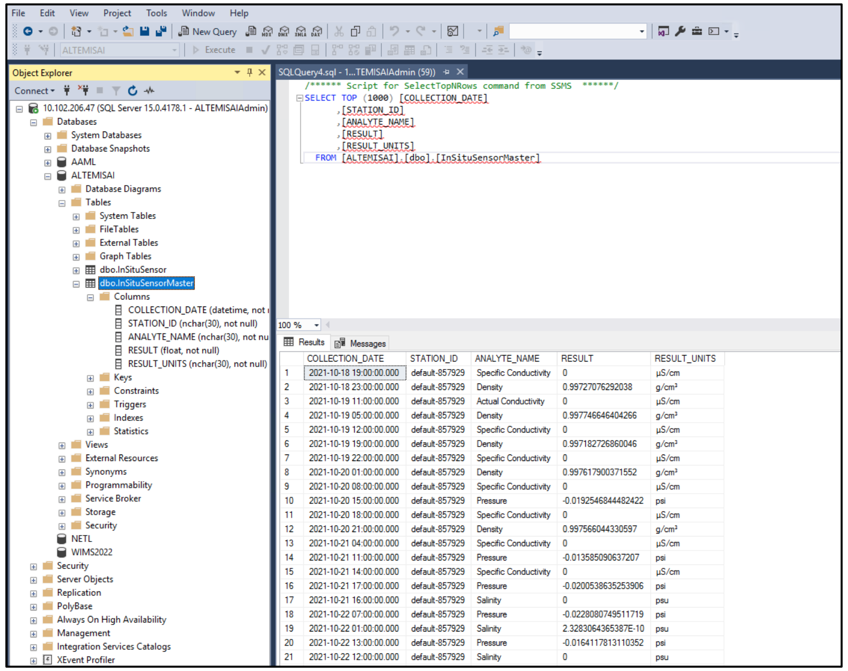
Data interfacing module development for the AI/ML System

FIU Year 2 Research Highlights:

- **Prototype data interfacing module development for the AI/ML System**
  - The sensor data from the ALTEMIS project will be available through an application programming interface (API) called HydroVu API.
  - Sensor collected variables will be water temperature, pH, specific conductance, and the water table (depth or DEPTH_TO_WATER).
  - To ensure that a reliable system is established for holding the latest in-situ sensor data, a SQL Server Database was created.
  - Once this data is secured on the database, it can be accessed from other systems and machine learning algorithms.

```python
for id, station_id in zip(locations.id, locations.name):
    last_tm = 0
    while(last_tm < yesterday):
        if(data.shape[0] == 0 and last_tm==0):
            last_tm = 0
        elif(data.shape[0] != 0 and last_tm==0):
            last_tm = 0
        else:
            last_tm = int(data['timestamp'].iloc[-1])
        try:
            print(last_tm)
            r = requests.get(url="https://www.hydrovu.com/public-api/v1/locations/{}/data?startTime={}".format(id, last_tm), headers=headers)
            parameters = pd.DataFrame(json.loads(r.text))
            params = pd.json_normalize(parameters['parameters'])[['parameterId', 'unitId', 'readings']]
            params = params.replace({"parameterId": param_unit_dict.parameters}).replace({"unitId": param_unit_dict.units})
            params = params.rename({"parameterId":"ANALYTE_NAME", "unitId":"RESULT_UNITS"}, axis=1)
            for i in range(params.shape[0]):
                curr = pd.DataFrame(params.readings[i])
                curr = curr.rename({"value":"RESULT"}, axis=1)
                curr['STATION_ID'] = station_id
                curr['ANALYTE_NAME'] = params.iloc[i]['ANALYTE_NAME']
                curr['RESULT_UNITS'] = params.iloc[i]['RESULT_UNITS']
                data = pd.concat([data, curr])
            last_tm = int(data['timestamp'].iloc[-1])
        except:
            print(count, "Resuming...")
            pass
```

Data interfacing for AI/ML system



InSitu Sensor Database in SQL server

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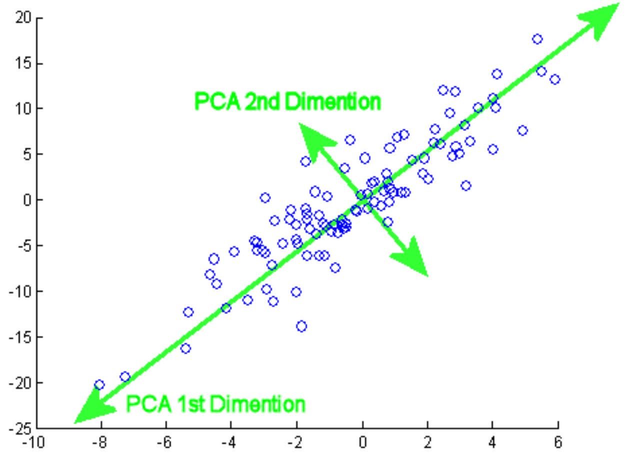
Development of the AI/ML based system to perform predictive analytics using datasets containing time-series and imagery data from sensors

FIU Year 2 Research Highlights:

- **Predictive analytics of time-series from sensors**
  - Principal Component Analysis (PCA) was applied on the dataset to determine the F-Area's master and proxy variables.
  - After the PCA, 95% variability explaining Principal Components (PC) were considered.
  - Each analyte's contributions are summed from different wells and analytes are ranked according to their sum of coefficients in the PCs.
  - This approach is still under investigation and was inconclusive in finding the proxy variables



Visual explanation of PCA

	PCA-1	PCA-2	PCA-3	PCA-4	PCA-5	PCA-6	PCA-7	PCA-8
AIR TEMPERATURE	0.102380	1.234097e-01	3.495543e-01	3.407639e-01	5.355415e-02	6.090447e-02	2.043845e-01	1.687024e-01
ALUMINUM	0.209404	1.531009e-01	2.450514e-02	7.022393e-02	2.330824e-02	2.133390e-02	3.254308e-02	5.290117e-02
ANTIMONY	0.226339	3.393170e-02	2.846445e-02	6.779185e-02	5.381069e-02	1.571567e-02	2.082037e-02	9.875431e-02
ARSENIC	0.216403	1.185710e-01	5.077209e-02	9.404089e-02	5.793076e-02	4.365579e-02	4.496003e-02	9.159309e-02
BARIUM	0.041901	4.228686e-01	4.763509e-02	6.188755e-03	5.170906e-02	9.015444e-02	1.165268e-01	8.270252e-02
CADMIUM	0.195584	1.390958e-01	2.088727e-01	1.322026e-01	4.113189e-02	2.964509e-02	2.358105e-02	2.215028e-02
CHROMIUM	0.227322	1.181977e-02	2.249990e-02	6.053330e-02	5.236909e-02	8.384730e-03	1.443588e-02	9.991355e-02
COBALT	0.196552	7.158359e-02	2.441781e-01	1.640933e-01	5.932134e-02	4.681411e-02	5.054937e-04	2.531334e-02
COPPER	0.208106	2.253234e-02	2.111304e-01	1.485372e-01	4.549500e-02	3.999765e-02	2.554200e-02	2.697470e-03
FLOW RATE	0.061055	4.099440e-01	8.782828e-02	6.388255e-02	5.706739e-02	4.528206e-02	3.095622e-02	6.287574e-02
GROSS ALPHA	0.201608	1.723345e-01	1.139024e-01	9.772754e-03	6.835300e-02	1.279833e-01	3.573303e-02	7.927211e-02
IODINE-129	0.145042	9.332004e-02	3.604424e-01	9.591866e-02	2.298940e-01	1.237840e-01	8.900711e-02	8.871691e-02
LEAD	0.192421	1.150853e-01	1.934076e-01	1.886733e-01	1.208674e-01	1.728585e-02	4.454083e-03	1.678293e-01
MERCURY	0.073673	4.137209e-02	3.881847e-01	4.241298e-02	1.522035e-01	3.265145e-01	4.354033e-01	7.049603e-02
NICKEL	0.201101	1.963278e-01	1.013251e-01	3.641300e-02	1.510642e-03	2.004341e-02	4.365913e-02	1.037564e-02
NITRATE-NITRITE AS NITROGEN	0.030262	2.686606e-01	1.908299e-02	2.929274e-01	2.281528e-01	5.235250e-01	2.254715e-01	1.619122e-01
NONVOLATILE BETA	0.212211	1.622360e-01	4.201748e-02	4.143243e-02	2.054718e-02	1.939661e-02	4.730751e-02	1.881391e-02
PH	0.198950	1.241813e-02	1.458567e-01	1.294656e-02	3.863705e-02	1.458886e-01	9.224930e-02	3.284768e-01
PHENOLPHTHALEIN ALKALINITY (AS CACO3)	0.000000	2.783329e-29	1.569284e-25	3.060726e-23	4.257709e-20	1.001991e-18	9.812416e-19	5.467697e-18
RADIUM-226	0.146314	2.565300e-01	1.930703e-01	1.003220e-01	2.229073e-01	1.516109e-02	9.797535e-02	1.188350e-01
RADIUM-228	0.017079	1.831709e-01	8.438320e-02	3.353698e-01	4.123578e-01	5.901668e-03	2.050289e-01	3.801160e-01
SELENIUM	0.213242	6.008249e-02	1.238945e-01	1.504982e-01	8.964931e-02	4.633820e-02	4.005977e-02	1.260389e-01
SILVER	0.214773	1.273973e-01	5.304807e-02	9.663064e-02	5.822603e-02	4.655779e-02	4.744864e-02	9.058450e-02
SPECIFIC CONDUCTANCE	0.020991	8.266471e-02	5.497949e-03	9.810204e-02	6.584954e-01	5.352365e-01	1.288482e-01	1.146437e-01
THALLIUM	0.193350	2.097446e-01	7.375532e-02	1.192460e-01	5.957249e-02	7.351090e-02	7.036592e-02	7.843054e-02

Sample PCA coefficients for the first 8 principal components at a specific well

Development of the AI/ML based system to perform predictive analytics using datasets containing time-series and imagery data from sensors

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FIU Year 2 Research Highlights:

- **Machine Learning (ML) model's prediction of contaminant concentrations using sensor collected variables**
  - Aqua Troll 200 and 500 sensors sense variables pH, reduction potential (RP), total dissolved solids (TDS), depth (DTW), specific conductance (SC), water temperature (WT).
  - Main contaminants of concern were Uranium-238, Iodine-129 and Tritium.
  - From the Pearson coefficient (PC) results, specific conductance (SC) and uranium-238 were selected to perform predictions as it had the highest correlation of 0.873.
  - With SC selected as the predictor and U-238 as the target variable, various ML models on the dataset were applied and their respective performance were evaluated.

	DEPTH_TO_WATER_FSB 95DR	IODINE-129_FSB 95DR	PH_FSB 95DR	SPECIFIC CONDUCTANCE_FSB 95DR	TRITIUM_FSB 95DR	URANIUM-238_FSB 95DR	WATER TEMPERATURE_FSB 95DR
DEPTH_TO_WATER_FSB 95DR	1.000000	0.238117	0.289611	-0.433384	-0.447817	-0.491157	-0.081103
IODINE-129_FSB 95DR	0.238117	1.000000	0.174478	-0.372613	-0.445152	-0.513656	0.047443
PH_FSB 95DR	0.289611	0.174478	1.000000	-0.518922	-0.529456	-0.554016	-0.005883
SPECIFIC CONDUCTANCE_FSB 95DR	-0.433384	-0.372613	-0.518922	1.000000	0.850204	0.872637	-0.102052
TRITIUM_FSB 95DR	-0.447817	-0.445152	-0.529456	0.850204	1.000000	0.936764	-0.080107
URANIUM-238_FSB 95DR	-0.491157	-0.513656	-0.554016	0.872637	0.936764	1.000000	-0.054804
WATER TEMPERATURE_FSB 95DR	-0.081103	0.047443	-0.005883	-0.102052	-0.080107	-0.054804	1.000000

Correlation matrix of the considered analytes

Mean Square Errors of each ML Model

ML Model	MSE
LinearRegression	0.005255
SGDRegressor	0.037348
KernelRidge	0.001665
BayesianRidge	0.005260
GradientBoostingRegressor	0.017442
SVR	0.014346

Development of the AI/ML based system to perform predictive analytics using datasets containing time-series and imagery data from sensors

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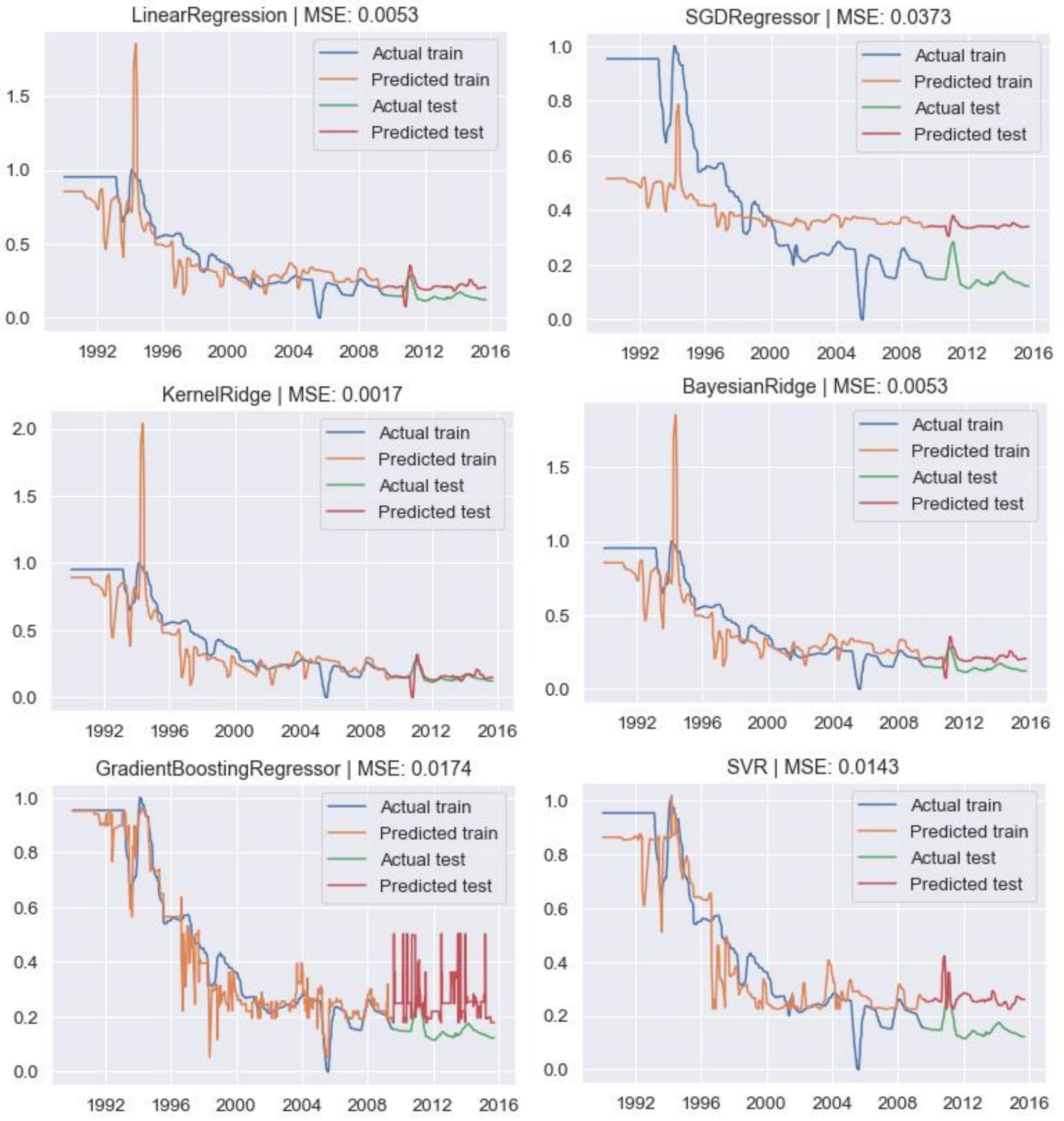
FIU Year 2 Research Highlights:

- **Machine Learning (ML) model's prediction of contaminant concentrations using sensor collected variables**
  - As is evident in the MSE results, kernel ridge regression performed the best giving an error of 0.0016 on the testing set
  - The prediction matches best the actual concentration in the plot
  - Although the results are according to the metric used for evaluation, most of the models did not generalize well on neither the training not testing set which assumed to be due to single feature used.



Training and testing predictions of each ML Model

Development of the AI/ML based system to perform predictive analytics using datasets containing time-series and imagery data from sensors

FIU Year 2 Research Highlights:

Deep Learning (DL) model's prediction

- DL models were tested to predict uranium-238 values using the four primary sensor collected variables: water temperature, pH, specific conductance, and the water table (depth or DEPTH_TO_WATER)
- The Deep Learning model is composed of several LSTM layers consisting of 25, 50, 100, 100 neurons respectively, followed by a dense layer of 25 neurons.
- the model takes in as input 60 previous values of each of the 4 input analytes for each well of the 25 wells and outputs a single value for the next time step for each of the 25 wells
- The results shown in the table are sorted from the best performing predictions to the worst results.

```
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 lstm (LSTM)                 (None, 60, 16)            10688

 lstm_1 (LSTM)               (None, 60, 32)            6272

 lstm_2 (LSTM)               (None, 60, 64)            24832

 lstm_3 (LSTM)               (None, 64)                33024

 dense (Dense)               (None, 25)                1625

=================================================================
Total params: 76,441
Trainable params: 76,441
Non-trainable params: 0
_________________________________________________________________
```

Deep Learning Model architecture

Mean Square Errors of the testing set for each well using the same DL model sorted from best to worst

Well name	MSE
FSB120D	0.003397
FSB 99D	0.004078
FEX 4	0.006953
FSB138D	0.007425
FSB116D	0.007883
FSB114D	0.014966
FSB135D	0.021066
FSB108D	0.022508
FPZ 6A	0.024303
FSB126D	0.025907
FSB 91D	0.028179
FSB130D	0.031664
FSB127D	0.031774
FSP204A	0.034619
FSB 95DR	0.055514
FPZ 6B	0.065643
FSB 79	0.081650
FPZ 4A	0.088865
FSB118D	0.096445
FSB 97D	0.099618
FPZ008AR	0.109162
FSB 78	0.111251
FSB132D	0.141650
FSB124D	0.150550
FSB128D	0.201747

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FIU Year 3 Projected Scope

- **Subtask 8.6: Publishing of AI/ML Models on the AAML System**
  - FIU will deploy the AI/ML models developed under this task towards the mission goal.
  - Several AI/ML models were developed previously for various purposes, mainly predicting contaminant concentrations into the future. For instance, identifying the master/proxy variables and optimization for sensor placement groundwater wells.
  - These models will be deployed by publishing them on an AAML system to be used by other sites and labs to solve similar problems. This will make access to these ML models easy to access and analyze.

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DOE EM IT/AI Deployment Roadmap

	Technology	2020	2021	2022	2023	2024
HQ All Sites	 WIMS	Site Deployment				
HQ, SRNL, ANL, PNNL	 KM-IT	Site Deployment				
HQ SRNL	AI D & D	Algorithm Development	AI System Development	In-house Deployment		
PNNL	AI Soil & Ground Water	Data Exploration/ Visualization	Algorithm Development	AI System Development & Integration	In-house Deployment	Site Deployment
LBNL, SRNL	AI Soil & Ground Water	Data Exploration & Visualization	Algorithm Development	AI System Development & Integration	In-house Deployment	Site Deployment
SRNL	AI Waste Process				AI System Development	In-house Deployment

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DOE-FIU Cooperative Agreement

Upcoming Events Announcement

DOE Fellows Poster Exhibition

DOE Fellows Induction Ceremony

Thank You. Questions?